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Reference Repository Definition Shale

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REFERENCE REPOSITORY DEFINITION

SHALE

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ABSTRACT

This report examines the geologic and hydrologic settings of three regions in North America as the basis for selection of one natural system to serve as a model for a reference repository system in shale (RRS-SH). In this RRS, shale is the candidate host medium for a high-level radioactive waste depository. The three regions studied are: (1) the Illinois Basin in Illinois, (2) the Williston Basin in South Dakota, and (3) the western Canada sedimentary basin in Alberta.

For each region, the configuration of the geologic media, the properties of the media that affect waste isolation, and the ground-water flow regime are described. These descriptions are used to evaluate the suitability of each system as a basis for RRS definition and to document the process by which the RRS was selected. The reference repository system in shale (RRS-SH) defined in this report is based on a portion of the western Canada sedimentary basin in southeastern Alberta, Canada. The reference repository, as herein defined, is not the representation of "average" values and characteristics for shale systems in general; it is the representation of an existing natural system in shale with its own unique combination of geometry, properties, and boundary conditions. The process of characterization of the selected natural system and the subsequent definition of the reference system based on it does not necessarily identify an "ideal" shale system; rather, this effort has produced a hypothetical reference system, with the important characteristics of a typical real shale system, on which a risk assessment methodology can be exercised.

From the region studied, a 150 kilometer by 1000 meter (vertical dimension) north-south cross section with six geologic units has been selected for use in ground-water modeling. A thick sequence of shales in the Upper Colorado Group (Upper Cretaceous) serves as the host unit. Ground-water flow in the RRS-SH is mostly horizontal through thin sandstone aquifers and downward through the host unit. Transport simulations were made for contaminant sources representing depositories located at two places in the system. For one location, contaminants move generally downward but remain confined in the host unit for times up to 135,000 years, in spite of appreciable spreading from the source. Very similar results are obtained for the other location. However, in this case the rate of spreading is much less because of decreased hydraulic gradients at that place in the flow domain. Both of the transport simulations indicate that, for the conditions which we have considered, contaminant confinement far in excess of 100,000 years is possible in this reference repository system.

SUMMARY

Reference repository system (RRS) definition is an integral part of the ongoing U.S. Nuclear Regulatory Commission program to develop and refine the methodology for assessment of risk associated with disposal of high-level radioactive waste in deep, excavated cavities in geologic media. Reference repository systems based on naturally occurring geologic and hydrologic systems provide a realistic basis for exercising the methodology on various geologic media in different settings. Application of the methodology in RRS analysis helps to establish the experience base needed for evaluation of risk associated with repository sites proposed in license applications submitted by the Department of Energy.

In this report, geologic systems in three regions of North America are examined to identify the system best suited as a model for the reference repository system in shale (RRS-SH). The three systems are: (1) the Illinois Basin in Illinois, (2) the Williston Basin in South Dakota, and (3) the western Canada sedimentary basin in Alberta, Canada. These were selected because the existing published and unpublished data base for each is most nearly adequate to provide for the detailed characterization of the ground-water flow regime and of the configuration and properties of the geologic media necessary for RRS definition.

The Illinois Basin is a deep structural basin in southern Illinois that is filled with up to 4300 meters of Paleozoic sedimentary rocks that consist of approximately equal thickness of shale, sandstone, and carbonate units. The candidate host unit in the sequence is the New Albany Shale Group (Upper Devonian). A deep, slowly moving ground-water system carries water from a recharge region at the margin of the basin down the structural dip toward the center of the basin, where discharge upward to the surface is probably localized along fractures associated with anticlinal structures and fault zones. The flow system is known mostly from studies of temperature and chemistry of basin waters. Measurements of hydraulic head are insufficient to determine the distribution of head in the basin, and the absence of this important aspect of the data base makes the Illinois Basin unacceptable as a model for the RRS-SH. However, an excellent data base exists on properties of the geologic units, and this will be used to supplement the data from other areas and to support decisions on values (and ranges of values) to be assigned to properties of units in the RRS-SH.

The Williston Basin in South Dakota contains a sequence of Paleozoic and Mesozoic sedimentary rocks dominated in the upper part by very thick Upper Cretaceous shale units. The shales are underlain by high-pressure artesian sandstone aquifers. Records of hydraulic head measurements taken as early as the 1890s are available in sufficient quantity to document a deep, regional ground-water flow system that was near natural equilibrium. Subsequent pumping of ground water has reduced aquifer pressures to the extent that the upward flow which existed within the Upper Cretaceous shales when the first wells were drilled has now been reversed, and today the flow is almost everywhere downward through the shales. The sensitivity of the flow system to exploitation of fluid resources and the lack of data for characterization of hydrologic properties of the geologic units makes this part of the Williston Basin a poor candidate for the RRS-SH. The former also emphasizes the importance of considering possible human influence on ground-water flow in repository systems.

The western Canada sedimentary basin in southeastern Alberta contains a sequence of Paleozoic and Mesozoic sedimentary rocks that, like the Williston Basin, is dominated in the upper part by thick Upper Cretaceous shales with some thin interbedded sandstones. For this study, we have compiled sufficient data to map the distribution of both hydraulic head and hydraulic conductivity of the principal aquifers in the basin. These data along with stable isotope analyses (deuterium and ^{18}O) for major aquifers allow detailed examination of ground-water flow in the basin. Because this information is available and because the configuration and properties of geologic units in the area are well known, the western Canada sedimentary basin has been selected as the model for the RRS-SH.

This report presents the results of the investigations that led to definition of the reference repository system in shale, and summarizes the important characteristics of that system. Specific topics treated are (1) the configuration of hydrogeologic units within the selected cross section, (2) the values and ranges of values for hydrologic, geochemical, thermal, and mechanical properties of the hydrogeologic units, (3) the boundary conditions selected for the cross section, (4) modeling results for the ground-water velocity field in the undisturbed system, (5) radionuclide attenuation mechanisms, and (6) geologic and non-geologic factors that influence repository performance. Emphasis has been placed on those characteristics that control ground-water flow in the undisrupted system. Other aspects, more important to performance of the disrupted system and scenario evaluation, have been identified but not treated in depth.

From the region studied in southeastern Alberta, a 150 kilometer by 1000 meter (vertical dimension) north-south cross section with six geologic units has been selected for use in the ground-water modeling. A thick sequence of shales in the Upper Colorado Group (Upper Cretaceous) serves as the host unit. Ground-water flow in the RRS-SH is mostly horizontal through thin sandstone aquifers and downward through the host unit. Transport simulations were made for contaminant sources representing depositories located at two places in the system. For one location, contaminants move generally downward but remain confined in the host unit for times up to 135,000 years, in spite of appreciable spreading from the source. Very similar results are obtained for the other location. However, in this case the rate of spreading is much less because of decreased hydraulic gradients at that place in the flow domain. Both of the transport simulations indicate that, for the conditions which we have considered, contaminant confinement far in excess of 100,000 years is possible in this reference repository system.

The present state of knowledge of the characteristics of shales and behavior of shales in the presence of radioactive wastes does not identify any feature or group of features of shales that make them unworthy of further consideration as a radioactive waste disposal medium.

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1. INTRODUCTION

1.1 Necessity of Reference Repository Definition to Risk Assessment Methodology

One of the principal objectives of research dealing with the management of high-level radioactive wastes is the assessment of risk associated with disposal of waste in deep, excavated cavities in geologic media. Evaluation of risk for such a geologic repository will require both a significant understanding of the waste disposal system and a systematic methodology for risk assessment that can be used for the evaluation. Because a repository does not currently exist, a reference system must be defined that has the important attributes of a geologic repository. The reference repository system (RRS) should have the important characteristics of a real system so that it can be effectively used for development of the risk assessment methodology and for development of insights into the behavior of systems based on different geologic media.

The principal characteristics of a reference repository are: (1) the spatial boundaries of the geologic system in which it is located; (2) the geometric configuration of the major rock units and geologic features within these boundaries; (3) the distribution of hydrologic, geochemical, thermal, and mechanical properties within the respective rock units; (4) the sources and distributions of potentials that affect ground-water movement within the system; (5) the boundary conditions of the system; (6) the characteristics of the excavation and civil structure; and (7) the waste emplacement package. In addition, a real geologic repository will have a history and a potential in the future for geologic and human activities that can affect the performance of the repository. These need to be identified and their possible influence evaluated.

Reference repository definition must proceed in a timely fashion. In the near future, license applications submitted to the Department of Energy for specific repository sites will need to be evaluated by the U.S. Nuclear Regulatory Commission. The methodologies developed and the experience gained during RRS analysis will be the basis for evaluation of risk associated with these repository sites. This report presents the definition of a reference repository system in shale (RRS-SH).

1.2 Natural Systems as the Basis for Reference Repository Definition

Because natural geologic systems are very complex the definition of a completely hypothetical reference repository is inappropriate, as it would be highly unlikely that a realistic system could be defined de novo. Instead, reference repositories need to be based on natural systems for which some data are available and for which some understanding already exists. In addition, the thorough examination of several natural systems as candidates for the reference repository system in a particular geologic medium not only broadens the data base from which values can be assigned to properties of geologic units in the system, but also increases the understanding of the complexity and variability of natural systems and of the processes and events that can affect them.

The systematic search which culminates with the identification of a natural geologic/hydrologic system to be used as the basis for a Reference Repository System (RRS) is similar to the process conducted by the Department of Energy in identifying appropriate sites for possible development of a geologic repository. Both exercises involve (1) identification of naturally occurring systems containing geologic and hydrologic characteristics potentially favorable for waste isolation, (2) screening of candidate systems through careful analysis of the available data base, and (3) detailed characterization of the specific system targeted as a possible reference repository or actual repository site. For the RRS, the specific natural system selected should be sufficiently representative of all such geologic systems that developed models and concepts will be generally applicable.

The principal decision in the selection of natural systems is that of rock type. Once the medium has been selected, other prerequisite features of the system should be those which generally characterize that particular type of geologic terrain. Certain features of the natural systems are of particular importance--for example, a closed or simple hydrologic system to facilitate modeling. A major consideration in the selection process is availability of information concerning the specific system. Knowledge of the geology and structure of the region is required in sufficient detail to define system boundaries and to characterize the rock mass. Data are needed on all features that could affect the system as a repository, including fracture and fault systems and the presence of dikes, as well as the history and possible reactivation of such features. An understanding of all important aspects of the hydrologic system is fundamental to meaningful modeling of potential flow and transport through the reference repository.

In targeting three natural systems for further study as candidates for the Reference Repository System in shale (RRS-SH), we have considered only those systems that contain shale units thicker than 60 m (about 200 ft) at depths of 300 to 1000 m (about 1000 to 3000 ft) below ground surface. The targeted systems each have an available data base judged potentially adequate for defining the configuration of geologic units and features and for characterization of the system hydrology. Only candidate systems having a basin hydrology potentially favorable for waste isolation were considered for additional study.

1.3 The Shale System as a Potential Waste Isolation System

As used in this report, the term "shale" refers to a large group of sedimentary rock types composed principally of clay-size (less than 4 microns) and silt-size (4-62 microns) particles. As rigorously defined in most geologic literature, shale has rather specific lamination or fissility parallel to the bedding. We will not restrict the term to its rigorous definition, but will use it in the broader sense to include claystone, siltstone, mudstone, lutite, argillite, and shale.

Shales are the most abundant type of sedimentary rock and probably form about half of the total volume of sedimentary rocks (Pettijohn, 1957). The mineralogic and chemical compositions and physical properties can differ markedly among shale deposits, and these reflect a diversity of sediment sources, depositional environments, and post-depositional histories.

Despite their abundance, shales are not as well studied as most other sedimentary rocks. Because of their fine-grained nature, shales are not easily disaggregated for mechanical analysis of particle size. Many of the constituents are not easily resolved under the microscope, and mineral identification must be accomplished by x-ray diffraction, chemical analysis, or other indirect means. Moreover, shales are generally not reservoir rocks for fluid or gaseous resources and therefore have not been subjected to the exhaustive study applied to the coarser and more permeable rock types.

Shales usually contain clay minerals, quartz, and calcite as their major constituents, but can contain a wide range of other minerals in the form of grains or cement. Clay minerals are largely responsible for the sorption capacity of shales, and consist of three major groups of related species--smectite, illite, and kaolinite. Each clay mineral group is characterized by a distinctive type of crystal structure, but has a considerable range of chemical composi-

tion. These groups vary greatly in their relative abundance in different shales and, because the groups have substantially different physical and chemical properties, their relative proportions in a given shale influence to a large degree its physical and chemical behavior. In general, the smectite and kaolinite groups are more abundant in younger shales. Smectite is generally absent in shales older than Mesozoic age (65 million yrs) and kaolinite is rare in rocks of pre-Devonian (395 million yrs) age. Most older shales contain illite as their dominant clay mineral.

Organic matter, often an important constituent of shales, occurs as fixed carbon or as bituminous hydrocarbons. Color can be an indicator of amount of organic matter present. Blacker shales generally contain more carbon, some in excess of 10 percent.

Natural geologic systems containing thick shale deposits offer a number of favorable features for the isolation of radioactive wastes. They also have some potentially unfavorable features. These are summarized in Table 1.1 and will be elaborated on in later sections of this report.

Table 1.1 Favorable and unfavorable features of the shale system as a waste isolation system

Potentially favorable features

1. Most abundant sedimentary rock type
2. Low intergranular and generally low fracture permeability
3. High clay mineral content for sorption of radionuclides
4. Plastic behavior under lithostatic load
5. Low solubility
6. Little or no resource value

Potentially unfavorable features

1. Heat induced alteration of clay minerals or organic matter
2. Mining and stability problems resulting from low strengths and plastic behavior
3. Presence of concentrated brines in some shales

2. SELECTION OF A NATURAL SYSTEM AS THE BASIS FOR THE REFERENCE REPOSITORY SYSTEM IN SHALE

2.1 Areas Considered and Reasons for Consideration

Three natural geologic systems were identified that sufficiently satisfy the general criteria for selection of candidate areas for the RRS-SH to warrant further detailed consideration. They are: (1) the Illinois Basin in Illinois, (2) the Williston Basin in central South Dakota, and (3) the western Canada sedimentary basin of southeastern Alberta, Canada (Figure 2.1). During the preliminary search for systems to be targeted for detailed examination, it was determined that each of these three areas contains thick shale units at the appropriate depths, and each has a substantial data base potentially adequate for characterization of media properties and configuration and for quantification of the ground-water flow system. Further, preliminary information on ground-water flow in the three basins suggested that each basin contains a flow system potentially favorable for waste isolation and, therefore, worthy of consideration as the model for the RRS-SH. The following sections discuss information compiled for the three basins, reasons for selection of the western Canada sedimentary basin as the basis for the RRS-SH, and specific aspects of the other two basins that help in defining a RRS-SH.

2.2 Illinois Basin

2.2.1 *Location and General Geologic Setting*

The Illinois Basin is a large spoon-shaped structural basin centered in southern Illinois and extending from the Mississippi River Arch and Ozark Dome on the west and south to the Cincinnati and Kankakee Arches on the east and north. Its central and deepest region is commonly referred to as the Fairfield Basin (Figure 2.2). The Illinois Basin underlies most of Illinois and parts of Indiana, Kentucky, and Missouri. Along its longest diameter it measures over 483 km (300 miles).

The region is drained by several major river systems, including the Mississippi, Illinois, Wabash, and Ohio Rivers. Surface topography in the region is flat to gently undulating. Topographic relief from the low areas at the center of the basin to the higher region around the basin perimeter ranges from 30 m (100 ft) to about 152 m (500 ft). The basin lies mostly within the Till Plains Section of the Central Lowlands physiographic province, and is within the area of North America that has been repeatedly covered by continental ice sheets during the last 1 to 2 million years.

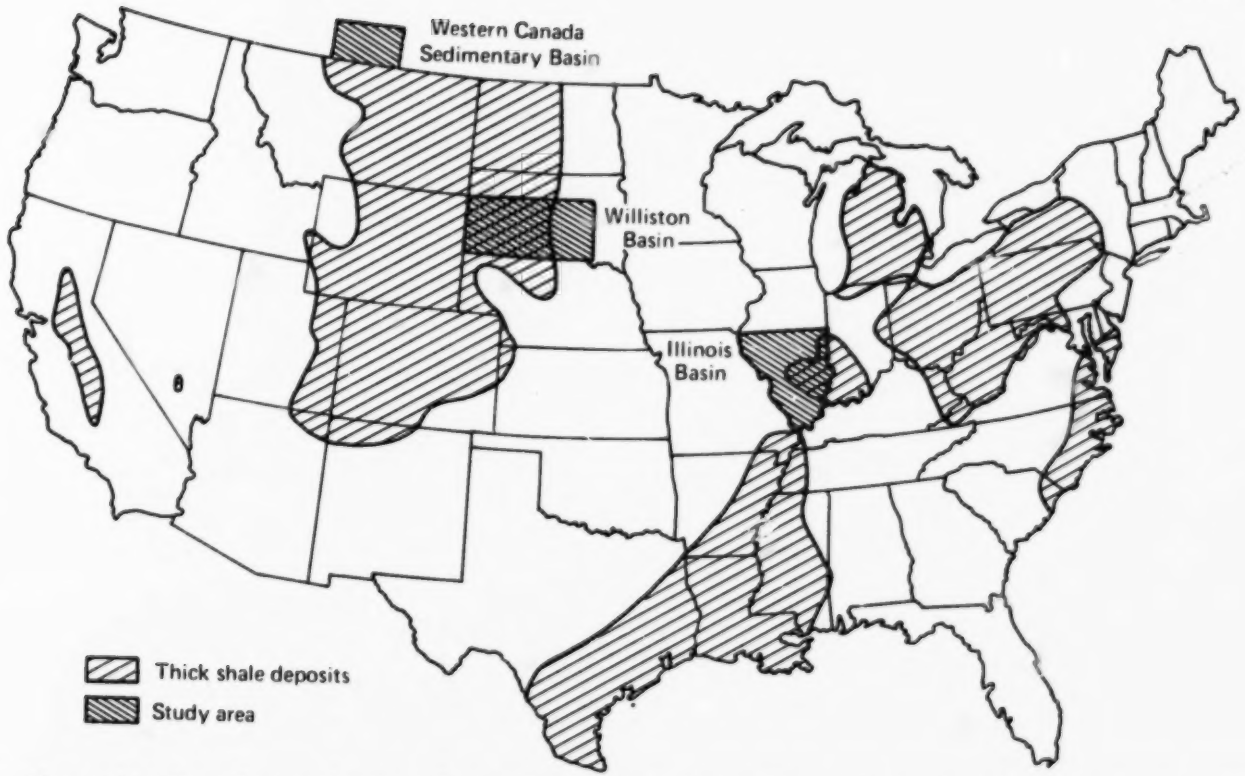

Figure 2.1 Map showing locations of thick shale deposits and principal study areas.

Figure 2.2 Map showing location of Illinois Basin with respect to major tectonic features.

The floor of the Illinois basin is formed by the Precambrian basement complex of igneous and metamorphic rocks, mostly granites and rhyolites. The top of the Precambrian ranges from elevation -610 m (-2000 ft) to -4267 m (-14,000 ft) below sea level. It is overlain by 914 m (3000 ft) to 4420 m (14,500 ft) of Paleozoic sedimentary rocks, mostly of marine origin. These rocks generally dip and thicken toward the center of the basin. With the exception of some of the deeper units, major rock units represented in the center of the basin also outcrop around the margin.

Rocks within the basin contain fossil fuel resources that have been exploited during the last 80 to 100 years. Geologic records, particularly from wells drilled for oil and natural gas, but also from coal exploration, water supply development and waste injection, provide a large data base for characterization of basin geology and hydrology.

In general, ground-water flow in the basin is from recharge areas in the peripheral outcrop belt, down the structural dip and toward the center of the basin, where flow is upward through the sedimentary rock sequence to produce surface discharge. Preliminary data that influenced selection of the Illinois Basin as a possible model for the RRS-SH indicated that the basin contained a slow-moving, deep ground-water system possibly favorable for waste isolation.

2.2.2 *Configuration of Geologic Units and Features*

Geologic units in the Illinois Basin have been studied by geologists and stratigraphers for more than 100 years, and the succession of sedimentary deposits represented in the basin has been extensively classified and subdivided. At present, over 700 stratigraphic names are applied to the sequence of rock units in the basin. For the purpose of ground-water studies and for characterization of the large-scale basin properties required for reference repository definition, these must be grouped into a smaller number of units on the basis of hydrologic properties and similarity of rock types. Many of the thin and/or areally restricted units can be combined with large units and ignored because of their lack of influence on the regional flow system. In addition, the large number of stratigraphic subdivisions that are based on color, fossil content, subtle bedding characteristics or mineralogic composition have little influence on gross water-conducting characteristics and are easily generalized into larger units. A grouping of rock units on the basis of lithologic

similarity, lateral continuity, thickness, and similarity of hydrologic properties provides the generalized stratigraphic column shown in Table 2.1. This column identifies thirteen units above the Precambrian. These units are discussed in greater detail in later sections, and are shown in cross section in Figure 2.6.

A geologic map of Illinois (Figure 2.3) shows the distribution of principal rock units beneath the cover of glacial drift. Youngest Pennsylvanian rocks outcrop in the center of the basin in southern Illinois, and successively older units are encountered toward the perimeter.

2.2.2.1 *Geologic Structure* - The locations of the major fault systems of northern and southern Illinois, the La Salle Anticlinal Belt, and other geologic structures in the basin are shown in Figure 2.4. The major tectonic structure in the basin is the La Salle Anticlinal Belt, the western edge of which is a relatively steep monoclinal slope that faces west. In places along it the strata have relief in excess of 610 m (2000 ft). Faulting accounts for only a minor part of the relief in the anticlinal belt, although deep-seated faulting in Precambrian rocks might account for the deformation of the overlying sedimentary rocks (Willman et al., 1975). A number of smaller anticlinal and monoclinal structures occur throughout the basin.

The sedimentary strata in southern Illinois near the center of the basin are broken by several large fault zones which trend NW-SE in southwestern Illinois, and NE-SW along the Wabash and Ohio River Valleys in southeastern Illinois. Most are normal faults that have displacements of a few hundred to a thousand feet (305 m). The last major tectonic movements which deformed rocks in the Illinois Basin probably occurred near the close of the Paleozoic Era several hundred million years ago.

The most intense deformation of rock strata in the Illinois Basin is not tectonic but is associated with the Glasford and Des Plaines Disturbances in northern Illinois (Figure 2.4). These features have been interpreted as disrupted zones caused by large meteorite impacts (Emrich and Bergstrom, 1962). The larger disturbance, the Des Plaines, has an area of about 65 km^2 (25 mi^2), and is crossed by numerous normal and reverse faults with displacements up to 183 m (600 ft). It was formed after Pennsylvanian time but prior to the most recent Pleistocene glaciation about

Table 2.1 Generalized geologic column for the Illinois Basin.

Unit*	Age	Dominant rock type	Thickness range (ft)
14. glacial drift	Quaternary	till	0 - 400
13. Pennsylvanian and Chesterian	Pennsylvanian and Mississippian	shale, sandstone, with some limestone and coal	0 - 3500
12. Mammoth Cave Limestone Megagroup	Mississippian	limestone	0 - 1000
11. Warsaw and Borden Formations	Mississippian	shale, siltstone	0 - 600
10. Fern Glen to Keokuk Formations	Mississippian	limestone	0 - 300
9. New Albany Shale Group	Mississippian and Devonian	shale	125 - 400
8. Hunton Megagroup	Devonian and Silurian	limestone	150 - 2000
7. Maquoketa Shale Group	Ordovician	shale	175 - 225
6. Ottawa Megagroup	Ordovician	limestone	300 - 1000
5. Ancell Group	Ordovician	sandstone	100 - 200
4. Knox Megagroup	Ordovician and Cambrian	dolomite	1100 - 4000
3. Eau Clair Formation	Cambrian	shale	400 - 1100
2. Mt. Simon Formation	Cambrian	sandstone	300 - 1300
1. Precambrian	Precambrian	granite	-

* List includes units of various stratigraphic ranking. Each unit is a composite of lesser units with similar rock types and hydrologic characteristics.

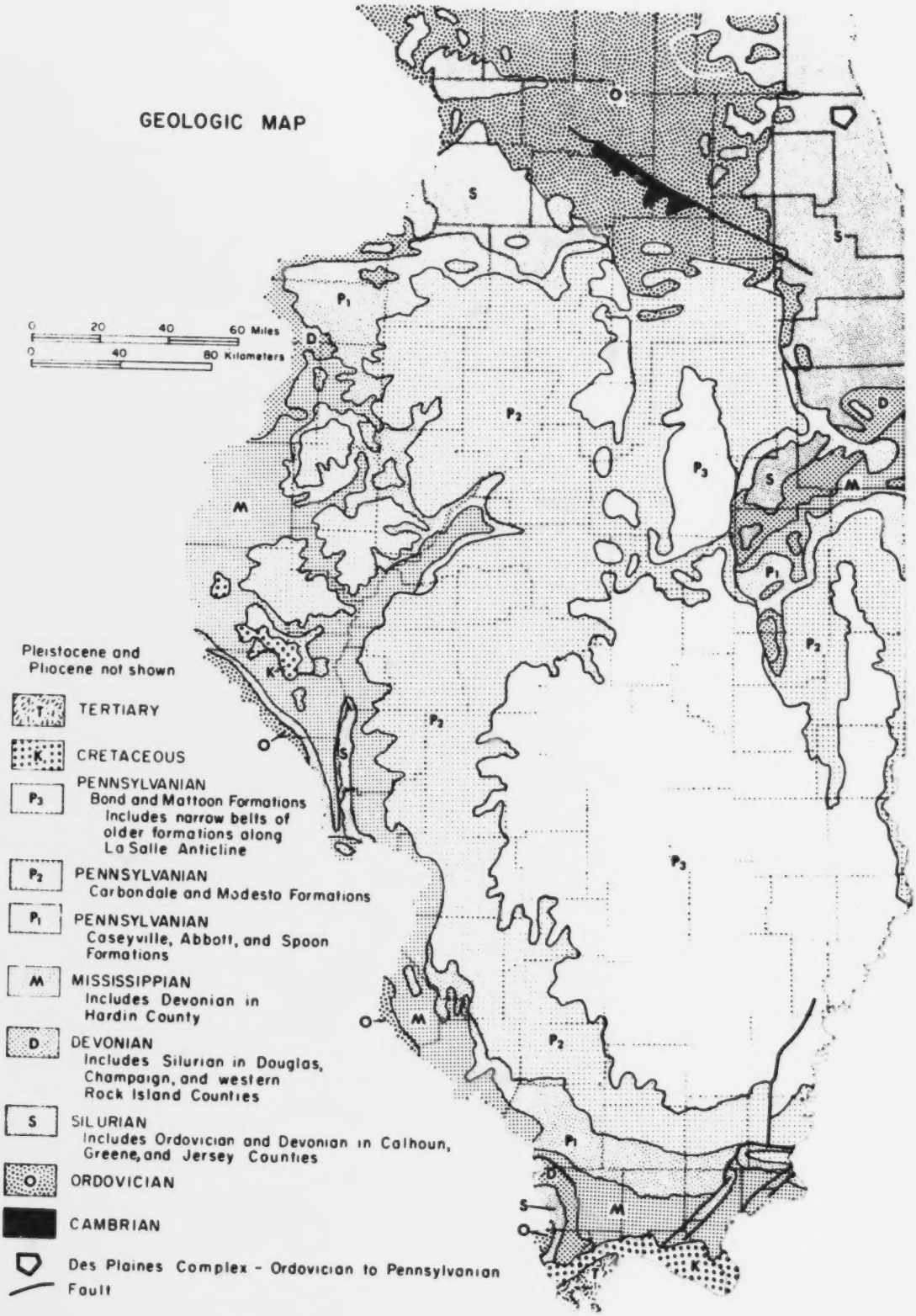
GEOLOGIC MAP
0 20 40 60 Miles
0 40 80 Kilometers
Pleistocene and Pliocene not shown
T TERTIARY
K CRETACEOUS
P3 PENNSYLVANIAN
Bond and Mattoon Formations
Includes narrow belts of older formations along La Salle Anticline
P2 PENNSYLVANIAN
Carbondale and Modesto Formations
P1 PENNSYLVANIAN
Caseyville, Abbott, and Spoon Formations
M MISSISSIPPIAN
Includes Devonian in Hardin County
D DEVONIAN
Includes Silurian in Douglas, Champaign, and western Rock Island Counties
S SILURIAN
Includes Ordovician and Devonian in Calhoun, Greene, and Jersey Counties
O ORDOVICIAN
CAMBRIAN
Des Plaines Complex - Ordovician to Pennsylvanian
Fault

Figure 2.3 Map showing the geology of the bedrock surface in Illinois (Willman and Frye, 1970).

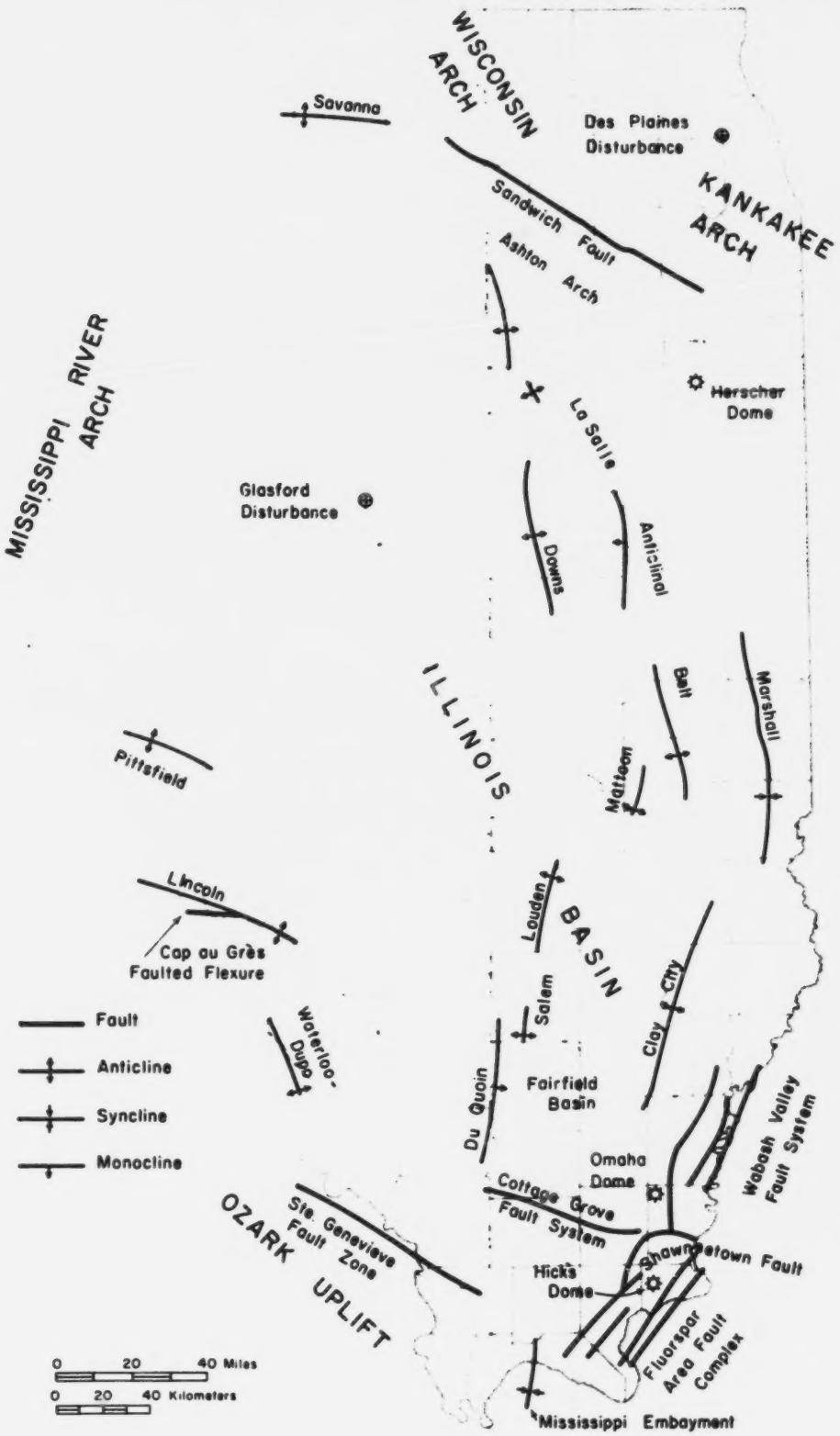

Figure 2.4 Map showing principal geologic structures of Illinois (Willman et al., 1975).

15,000 years ago (Buschbach and Heim, 1972). In the Des Plaines Disturbance, a disrupted zone at least 457 m (1500 ft) thick is preserved and an additional 305 m (1000 ft) or more of disrupted strata have been removed by erosion since the impact.

The structural depression of the center of the Illinois Basin, formed by repeated subsidence during the Paleozoic, is depicted in Figure 2.5. The Galena Group on which the structure contours in Figure 2.5 are drawn is the uppermost unit of the Ottawa Megagroup (Table 2.1). Strata above and below the Galena show the same general trend in structural dip toward the center of the basin (Figure 2.6).

2.2.2.2 *Description of Geologic Units* -
Precambrian rocks are not exposed within the basin and have been penetrated only at great depths by twenty borings. Samples recovered from the Precambrian basement complex are mostly granitic but include some granodiorite and rhyolite. Closely spaced borings in western Illinois indicate that local relief on the Precambrian surface might be several hundred feet.

In most of the basin, Cambrian sandstones included in the Mt. Simon Sandstone rest with major unconformity on the Precambrian igneous rocks. The Mt. Simon ranges up to 762 m (2500 ft) thick in northeastern Illinois but is generally thinner in the southern part of the state (Figure 2.6). It consists of fine to coarse grained, in places pebbly, friable sandstone composed mostly of quartz. In its lower part it contains large quantities of feldspar derived from underlying rocks. The Mt. Simon is an important aquifer in northeastern Illinois, but loses much of its porosity and contains highly mineralized water in the central and southern parts of the state.

The Eau Clair Formation is a unit of Cambrian age that overlies the Mt. Simon Sandstone and, in order of decreasing abundance, consists of shale, dolomite, sandstone, and limestone (Bell et al., 1964). It ranges from about 91 m (300 ft) to more than 305 m (1000 ft) thick and becomes more dolomitic toward the center of the basin. It is shown as a shale unit on Figure 2.6.

The Knox Dolomite Megagroup, as used here, overlies the Eau Clair Formation and is overlain by the Ancell Group (Figure 2.6). It consists of relatively pure dolomite and is the thickest unit identified in the Illinois Basin. In the center of the basin it exceeds 1219 m (4000 ft) but thins

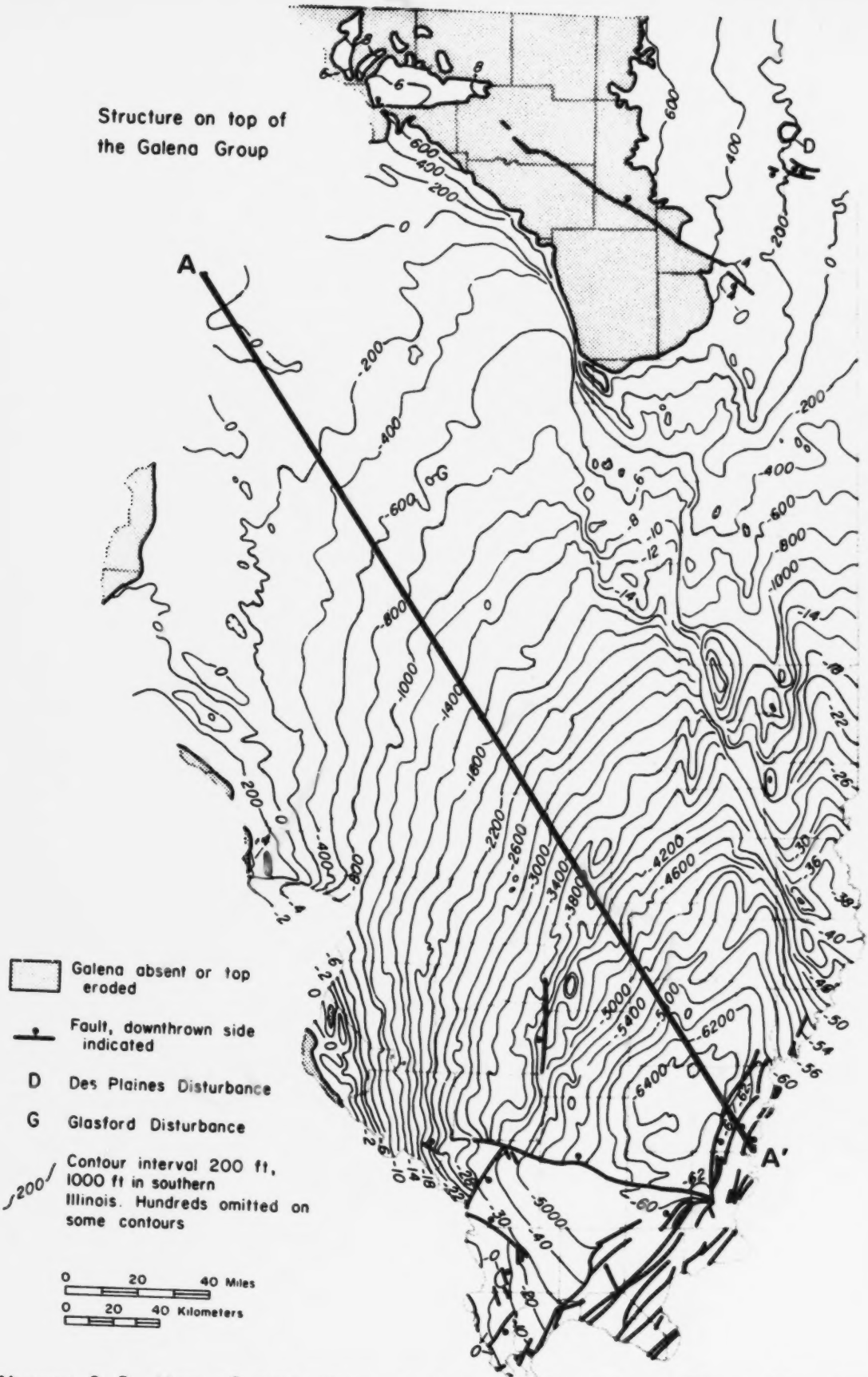
Structure on top of the Galena Group
A
A'
G
Galena absent or top eroded
Fault, downthrown side indicated
D Des Plaines Disturbance
G Glasford Disturbance
200 Contour interval 200 ft, 1000 ft in southern Illinois. Hundreds omitted on some contours
0 20 40 Miles
0 20 40 Kilometers

Figure 2.5 Map of structure on top of the Galena Group (Ottawa Megagroup) (Willman et al., 1975). Datum is sea level.

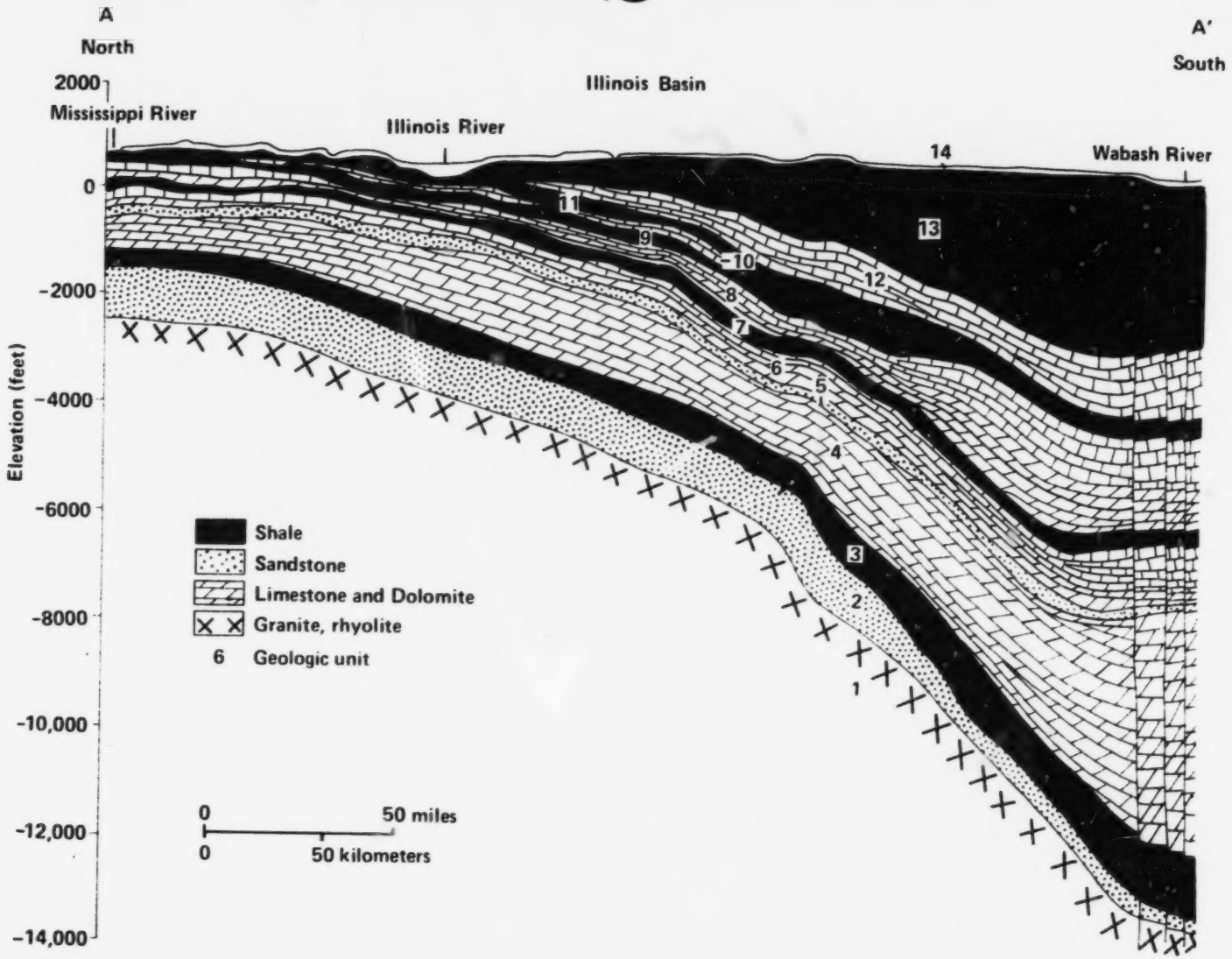

Figure 2.6 Diagrammatic cross section of Illinois Basin showing principal geologic units listed in Table 2.1. Location of section shown on Figure 2.5.

northward, mostly as a result of erosive truncation on the unconformity at its top. The Knox includes dolomites of Cambrian as well as Ordovician age. Some thin but highly permeable sandstones (i.e., the Ironton and Galesville Sandstones) present at the base of the Knox Megagroup are important aquifers in northern Illinois, but these become progressively more dolomitic and, consequently, less permeable and porous to the south.

The Ancell Group unconformably overlies the Knox Megagroup throughout most of the basin (Figure 2.6). It is entirely of Ordovician age, consists mainly of fine grained, poorly cemented, pure quartz sandstone with some minor shale and carbonate beds. It rarely exceeds 91 m (300 ft) in thickness and is a major aquifer where it occurs at shallow depths in northern Illinois.

The Ottawa Limestone Megagroup consists of the Middle Ordovician carbonate rocks overlying the Ancell Group and underlying the Maquoketa Shale Group (Figure 2.6). It is present throughout most of the basin and thickens from about 91 m (300 ft) in northern Illinois to 396 m (1300 ft) in the south. Several zones within the Ottawa Megagroup have yielded large volumes of oil and natural gas.

The Maquoketa Shale Group is one of the two shale units that could be considered a potential host medium for a reference repository based on the Illinois Basin. The Maquoketa is an Upper Ordovician unit consisting of two thick shale beds separated by a thin and discontinuous limestone bed. It ranges in thickness from about 46 m (150 ft) to nearly 107 m (350 ft). For two reasons, the Maquoketa was considered the less desirable of the two possible host units. First, its thickest areas occur in the deepest part of the basin below depths that could be considered for a depository, and second, the data base for the Maquoketa is rather restricted.

The Hunton Limestone Megagroup includes dominantly carbonate rocks of Devonian and Silurian age that lie between the Maquoketa Shale Group and the late Devonian to Mississippian New Albany Shale Group (Figure 2.6). The unit occurs throughout the Illinois Basin and attains a maximum thickness of over 549 m (1800 ft) near the center of the basin. In much of central Illinois it contains highly mineralized waters and has produced substantial quantities of petroleum.

The New Albany Shale Group is considered the most reasonable candidate host rock for a reference repository based on the Illinois Basin. The New Albany ranges in thickness from less than 30 m (100 ft) to over 122 m (400 ft), as

shown in Figure 2.7. Areas of 122 m (400 ft) or more are restricted to the deepest parts of the basin; however, shale beds thicker than 61 m (200 ft) and ranging in depth from 305 m (1000 ft) to about 488 m (1600 ft) occur on the western flank of the basin in central Illinois. The New Albany consists of an essentially continuous body of Middle and Upper Devonian and Lower Mississippian black, gray, and green shale. Darker color frequently corresponds to higher organic matter content, which in the New Albany ranges up to about 15 percent by weight in some areas. Through most of the western part of the Illinois Basin the New Albany is mostly gray shale. The New Albany and its equivalents in the Appalachian and Michigan Basins have been the subjects of intensive study in recent years by ERDA and now the DOE. The aim of the studies has been to evaluate the natural gas resource value of the low permeability reservoirs and to develop technologies for enhancement of gas production. The studies are extremely valuable to the present aim of quantification of shale systems, because they examine shale properties seldom studied in such detail (DOE, 1978).

On the western flank of the Illinois Basin the New Albany Shale Group is overlain by a sequence of shallow water marine carbonate rocks which terminate abruptly to the east (Figure 2.6). There, they are overlapped and replaced by thick gray deltaic siltstones and shales that overlie the New Albany in the central part of the basin (Lineback, 1966). The shallow marine carbonates, with an aggregate thickness of 30 m (100 ft) to 107 m (350 ft), belong to the Fern Glen Formation (at the base), the Keokuk Limestone, and the Burlington Limestone (Figure 2.6). These units were deposited on a shallow marine shelf west of a large Lower Mississippian delta. The deltaic siltstones and shales and the shales that overlap the Fern Glen to Keokuk interval and extend nearly to the western margin of the basin are included in the Borden and Warsaw Formations, respectively. The Borden which comprises the bulk of the deltaic sediments, exceeds 183 m (600 ft) in thickness in some areas. Where it directly overlies the New Albany in southern Illinois, the Borden and the New Albany together form a single shale unit over 244 m (800 ft) thick (Figure 2.6).

Overlying the Borden and Warsaw Formations is a succession of limestone groups and formations of Mississippian age that are included in the Mammoth Cave Limestone Megagroup. These relatively pure limestones diminish in thickness from nearly 610 m (2000 ft) in southern Illinois to little more than 30 m (100 ft) in eastern Illinois. They crop out extensively along the Mississippi and Illinois Valleys in western Illinois (Figure 2.3).

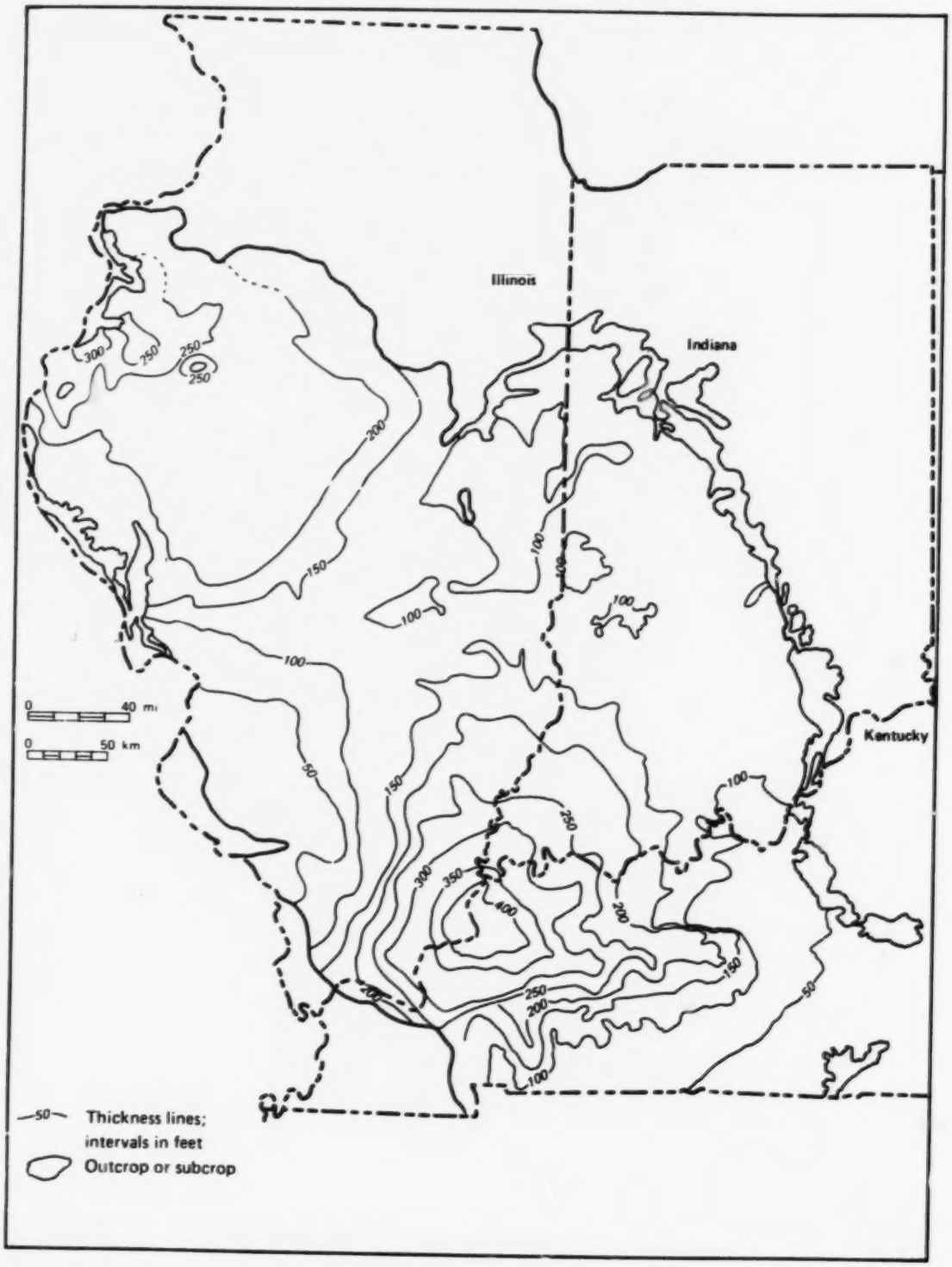

Figure 2.7 Map showing thickness of the New Albany Shale Group in the Illinois Basin (Barrows et al., 1979).

The uppermost bedrock unit listed in Table 2.1 and shown on Figure 2.6 includes strata belonging to the Chesterian Series (Mississippian) and the Pennsylvanian System. This unit probably contains a larger variety of rock types than any of the other units, but it is characterized by such thin strata and such extreme vertical variability in rock type that individual lithologic units have not been distinguished in this report. The unit contains shale as its most abundant rock type, but it also includes much limestone, sandstone, and coal. In general, sandstones are more common in the lower part and shale more abundant upward. Sandstones of the lower Pennsylvanian and Chesterian are the principal petroleum reservoir rocks in the Illinois Basin.

Glacial drift overlies most of the Illinois Basin except for its extreme southern part. During the Pleistocene Epoch glaciers repeatedly invaded the region, depositing glacial till, sand, gravel, and silt. The drift ranges from 0 to over 122 m (400 ft) thick and consists mostly of glacial till. Some thin sand and gravel zones in the drift yield substantial quantities of ground water.

2.2.3 *Properties of Geologic Units*

The waste isolation capability of a particular geologic medium is determined to a large degree by the hydrologic, geochemical, thermal, and mechanical properties of that medium and of the geologic system in which the medium is situated. Substantial data are available for the characterization of properties of geologic units in the Illinois Basin. The data base is discussed here and will serve as a basis for comparison with units in other areas studied.

2.2.3.1 *Hydrologic Properties* - Hydraulic conductivity and porosity (effective porosity) values for geologic units in the Illinois Basin are summarized in Tables 2.2 and 2.3. For the most part, these data are from laboratory analyses of core samples. Most of the non-shale samples are from oil reservoir rocks, aquifers, or zones used for natural gas storage. Consequently, the data base for sandstone, limestone, and dolomite is probably somewhat biased toward higher conductivities and porosities than would be found if all basin rocks had been sampled. This bias is especially noticeable in data for limestone and dolomite units which usually have lower porosity and lower conductivity than shown in Tables 2.2 and 2.3. Oil reservoirs in carbonate rocks in the basin occur mainly in zones that are fractured, are oolitic, or are solution channeled. Large thicknesses of carbonates yield little or no fluid and can

Table 2.2 Hydraulic conductivity values for geologic units in the Illinois Basin.

Unit	HYDRAULIC CONDUCTIVITY Mean ft/day	Mean cm/sec	Range ft/day	Range cm/sec	n	Reference
Penn. sandstones			0.33 - 1.2	1.2×10^{-4} - 4.2×10^{-4}		Bergstrom, 1968
Penn. sandstones	0.49	1.7×10^{-4}				Mast, 1967
Penn. sandstones	0.30	1.1×10^{-4}				Mast, 1967
Penn. sandstones	0.49	1.7×10^{-4}	0.03 - 3.9	1.2×10^{-5} - 1.37×10^{-3}	165	data from Van Den Berg, 1980
Penn. shale	5.5×10^{-9}	1.9×10^{-12}			1	Gonduin et al., 1958
Penn. shale	2.5×10^{-7}	8.7×10^{-11}			1	Gonduin et al., 1958
Chesterian sandstones			0.19 - 0.63	6.6×10^{-5} - 2.2×10^{-4}		Bergstrom, 1968
Chesterian sandstones	0.30	1.1×10^{-4}				Mast, 1967
Chesterian sandstones	0.25	8.7×10^{-5}				Mast, 1967
Chesterian sandstones	0.35	1.3×10^{-4}	0.01 - 8.22	4.8×10^{-6} - 2.9×10^{-3}	286	data from Van Den Berg, 1980
Mammoth Cave Ls. mg.	0.71	2.5×10^{-4}				Mast, 1967
Mammoth Cave Ls. Mg.	0.46	1.6×10^{-4}				Mast, 1967
Mammoth Cave Ls. Mg.	1.06	3.7×10^{-4}	0.005 - 8.23	1.9×10^{-6} - 2.9×10^{-3}	62	data from Van Den Berg, 1980
Warsaw and Borden sh.	0.03	1.1×10^{-5}			1	data from Van Den Berg, 1980
Fern Glen to Keokuk ls.	0.56	2.0×10^{-4}				Bergstrom, 1968
New Albany Sh. Gr.	1.9×10^{-6}	6.8×10^{-10}				Kalyoncu et al., 1978
New Albany Sh. Gr.	2.7×10^{-4}	9.7×10^{-8}				Hilton, 1978
Hunton Mg. ls. & dol.	0.13	4.6×10^{-5}				Mast, 1967
Hunton Mg. ls. & dol.	0.36	1.3×10^{-4}	0.05 - 1.17	1.7×10^{-5} - 4.1×10^{-3}	10	data from Van Den Berg, 1980
Maquoketa Gr. sh.	1.3×10^{-4}	4.6×10^{-8}				Walton, 1960
Ottawa Mg. dol.	0.13	4.6×10^{-5}				Mast, 1967
Ottawa Mg. dol.	0.04	1.3×10^{-5}	0.01 - 0.07	2.9×10^{-6} - 2.6×10^{-5}	3	data from Van Den Berg, 1980
Ancell Group ss.			0.37 - 1.10	1.3×10^{-4} - 3.9×10^{-4}		Bergstrom, 1968
Ancell Group ss.	1.38	4.8×10^{-4}	0.38 - 3.34	1.3×10^{-4} - 1.2×10^{-3}	4	data from Van Den Berg, 1980
Knox Mg. ss.			1.20 - 2.10	4.3×10^{-4} - 7.5×10^{-3}		Bergstrom, 1968
Knox Mg. ss.			3.76 - 6.01	1.2×10^{-3} - 1.9×10^{-3}		Hughes et al., 1966
Knox Mg. ss.	1.28	4.5×10^{-4}	0.67 - 1.93	2.4×10^{-4} - 6.8×10^{-4}	4	data from Van Den Berg, 1980
Eau Clair Fm. dol.	0.97	3.4×10^{-4}	0.41 - 1.52	1.4×10^{-4} - 5.4×10^{-4}	2	data from Van Den Berg, 1980
Mt. Simon Sandstone	1.34	4.7×10^{-4}				Walton and Csallany, 1962
Mt. Simon Sandstone	2.40	8.5×10^{-4}				Hughes et al., 1966
Mt. Simon Sandstone			0.027 - 0.15	9.7×10^{-6} - 5.3×10^{-5}		Bergstrom, 1968
Mt. Simon Sandstone	0.21	7.4×10^{-4}	0.04 - 0.51	1.4×10^{-5} - 1.8×10^{-4}	9	data from Van Den Berg, 1980

Table 2.3 Porosity values for geologic units in the Illinois Basin.

Unit	POROSITY Mean percent	Standard Deviation percent	Range percent	n	Reference
Penn. sandstones			17 - 20		Bergstrom, 1968
Penn. sandstones	19	1			Mast, 1967
Penn. sandstones	19	1			Mast, 1967
Penn. sandstones	19	3.0	12 - 40	171	data from Van Den Berg, 1980
Chesterian sandstones			16 - 18		Bergstrom, 1968
Chesterian sandstones	18	1			Mast, 1967
Chesterian sandstones	18	1			Mast, 1967
Chesterian sandstones	17	2.5	10 - 23	327	data from Van Den Berg, 1980
Mammoth Cave Ls. Mg.	15	1			Mast, 1967
Mammoth Cave Ls. Mg.	16	1			Mast, 1967
Mammoth Cave Ls. Mg.	14	2.6	6 - 20	85	data from Van Den Berg, 1980
Warsaw and Borden sh.	16			1	data from Van Den Berg, 1980
Fern Glen to Keokuk ls.	17				Bergstrom, 1968
New Albany Sh. Gr.	1.5	1.3	0.5 - 5.1	11	Kalynocu, 1978
New Albany Sh. Gr.			0.1 - 13		DOE, 1978
Hunton Mg. ls. & dol.	13	2			Mast, 1967
Hunton Mg. ls. & dol.	14	2.2	12 - 18	13	data from Van Den Berg, 1980
Maquoketa Sh. Gr.	NO DATA				
Ottawa Mg. dol.	13	2			Mast, 1967
Ottawa Mg. dol.	8	2.1	4 - 10	7	data from Van Den Berg, 1980
Ancell Group ss.			14.6 - 18.4		Bergstrom, 1968
Ancell Group ss.	16	1.6	14 - 18	4	data from Van Den Berg, 1980
Knox Mg. ss.			17.8 - 19.8		Bergstrom, 1968
Knox Mg. ss.	17	1.1	15 - 18	4	data from Van Den Berg, 1980
Eau Clair Fm. dol.	18		17 - 19	2	data from Van Den Berg, 1980
Mt. Simon ss.			10 - 13		Bergstrom, 1968
Mt. Simon ss.	12	1.6	10 - 15	9	data from Van Den Berg, 1980

be expected to have conductivities one or two orders of magnitude lower than those shown in Table 2.2. Porosities of carbonate rocks shown in Table 2.3 are generally lower than sandstone porosities, yet the average conductivities (Table 2.2) are equal to or higher than the sandstones. This observation might support the suggestion that fluid flow in the reservoir carbonates is principally through fractures or channels rather than through intergranular or intercrystalline porosity. No other information is available that might help quantify fracture porosity in units in the basin.

In general, both hydraulic conductivity and porosity show a decrease with increasing depth and increasing age of rocks in the basin. However, the magnitude of this decrease is less than the normal variation between rock types. Some of the highest mean conductivities occur in deep basin rocks--e.g., the Ancell Group (sandstone), Knox Megagroup (dolomite), and Mt. Simon Sandstone (Table 2.2).

Where the data base is sufficiently large, the frequency distribution of hydraulic conductivity and porosity measurements for individual geologic units can be examined (Figure 2.8). These data show that porosity is a normally distributed parameter exhibiting in most cases a nearly symmetrical bell-shaped distribution. Hydraulic conductivity is log normally distributed. Unfortunately, data sufficient to quantify these distributions are not available for most geologic units.

Shale units in the basin have a smaller data base than other units. In spite of this, the mean hydraulic conductivity values reported for shales in the basin (Table 2.2) range from 1.9×10^{-12} cm/sec to 9.7×10^{-8} cm/sec and closely approximate the limits of the range of conductivity considered typical for shales (Freeze and Cherry, 1979). Data on shale porosities are reported only for the New Albany Shale Group, and these analyses are from black shales that contain substantial quantities of kerogen, a light hydrocarbonic solid, that occupies a substantial portion of the pore volume and restricts the measured porosity. Thus, the 1.5 percent mean porosity (Table 2.3) for the New Albany reported by Kalyoncu et al. (1978) is probably much lower than can be expected in most non-organic shales.

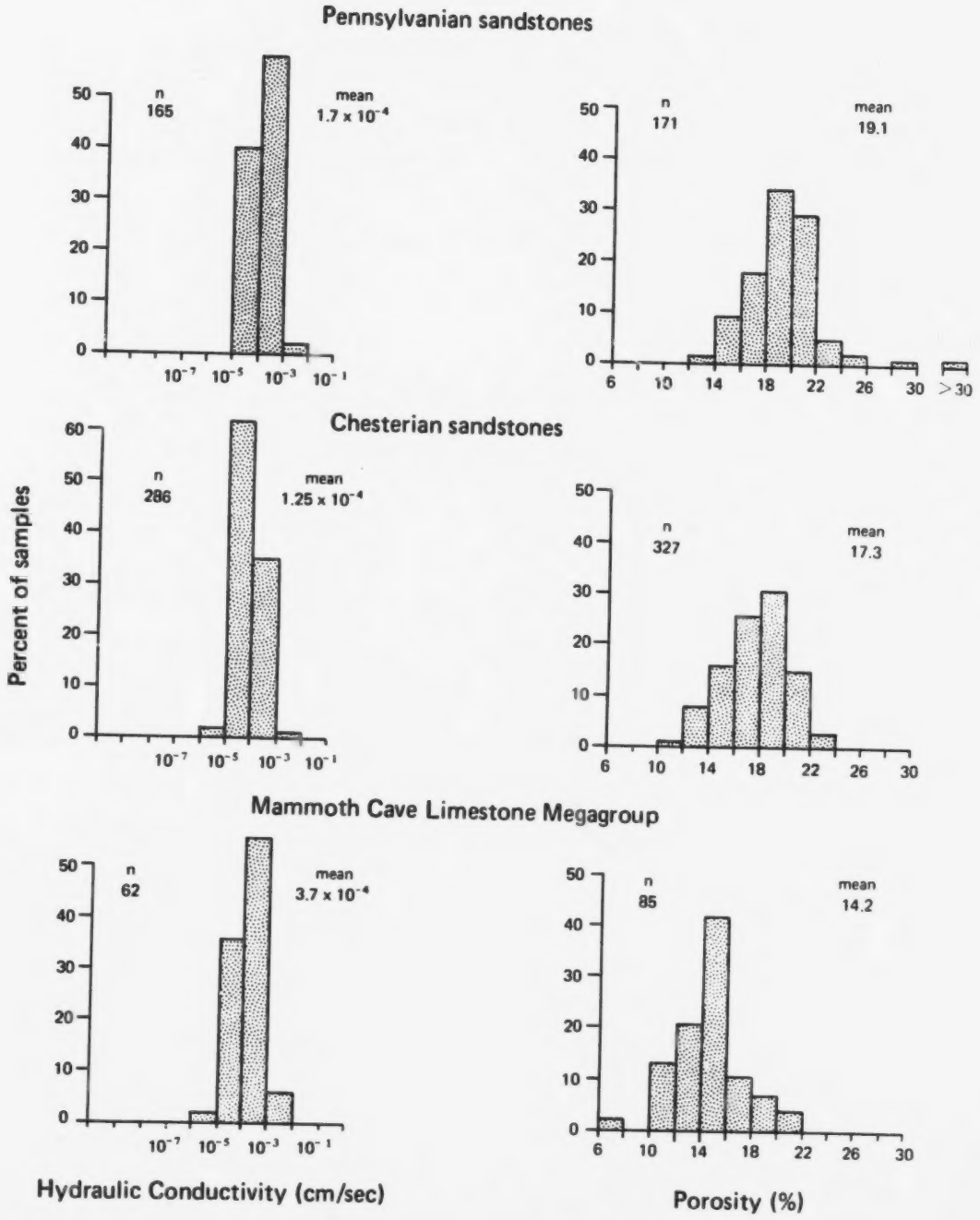

Figure 2.8 Histograms of hydraulic conductivity and porosity of geologic units in the Illinois Basin.

2.2.3.2 *Geochemical Properties* - The capacity of a system of sedimentary rocks to limit the migration of radionuclides from high level radioactive waste depends to a large degree on the type and amount of clay minerals present in the system, because these minerals contribute most to the sorption capacity of the system. Clay minerals present in shales in the Illinois Basin are mostly illite with some chlorite, kaolinite, and mixed-layer clays and minor amounts of smectite. All the non-shale units also contain clay minerals, probably of the same type found in the shales, but in lesser quantity.

Data on exchange capacity or distribution coefficient (Kd) that would quantify the sorption capacity of Illinois Basin shales for specific radionuclides are not available. However, detailed mineralogical and chemical characterization studies of shales and other units have been conducted (Armon and Rees, 1960; Grim et al., 1957; Harvey et al., 1977; Lamar, 1957; Stevenson and Dickerson, 1969), and from these studies, some general conclusions can be reached about the sorption capacity of shale in the Illinois Basin. The typical mineralogical composition of black shale from the New Albany Shale Group consists of quartz (40%), illite (40%), chlorite, and kaolinite. Trace minerals include pyrite, calcite, dolomite, and feldspar. Most other Illinois shales have similar clay mineral compositions and are also mostly illitic. In general, illite has a cation exchange capacity higher than kaolinite, about the same as chlorite, and much lower than smectite or vermiculite. Thus, the illitic Illinois shales might be expected to have a lower sorption capacity than more vermiculitic shales or smectite-rich shales.

The list of trace elements common in black shale from the New Albany Shale Group usually includes U, Th, Ti, Ba, and Bo. The black shale also typically contains 10 to 15 percent organic matter (Hilton, 1978). A number of studies of Devonian black shales have reported a highly significant correlation between organic carbon and U content, suggesting that soluble uranium compounds in transport in ground water are precipitated in the presence of or complexed with organic matter in the black shale (Swanson, 1961; Leventhal and Goldhaber, 1978). Uranium contents of 1 to 38 ppm and thorium contents of 1 to 16 ppm have recently been reported for the New Albany Shale (Leventhal and Goldhaber, 1978).

2.2.3.3 *Thermal Properties* - Thermal conductivity, heat capacity, and thermal expansion characteristics of geologic media plus the natural geothermal load determine the response of a host system to the thermal load added by burial of high level radioactive waste. The few available

published estimates of the thermal conductivity of Illinois Basin rocks are compiled in Table 2.4.

Data on thermal expansion of shales is not available from the Illinois Basin. Low temperature, 20 to 80°C (68 to 176°F) thermal expansion characteristics of Illinois limestone and dolomites reported by Harvey (1967) indicate that most coarse-grained dolomites and limestones expand more in a direction perpendicular to their bedding than parallel to it. Many fine-grained limestones expand more in a direction parallel to the bedding. Values for the coefficient of thermal expansion range from $4.0 \times 10^{-6}/^{o}C$ to $1.8 \times 10^{-5}/^{o}C$ for limestone and from $5.6 \times 10^{-6}/^{o}C$ to $1.1 \times 10^{-6}/^{o}C$ for dolomite. Average values are $7.7 \times 10^{-6}/^{o}C$ for limestone and $9.4 \times 10^{-6}/^{o}C$ for dolomite.

The ambient temperature in the vicinity of a depository placed between 300 m and 1000 m in the Illinois Basin can be estimated from the natural geothermal gradient and average annual surface temperature. The thermal gradient in the basin has been measured at 19.5°C per kilometer (McGinnis, 1968), and the surface temperature averages about 12.8°C. Thus, temperatures in the vicinity of a depository prior to waste emplacement could be expected to range from about 18.9°C to about 32.3°C at depths between 300 m and 1000 m.

2.2.3.4 *Mechanical Properties* - Few data are available for mechanical properties of individual geologic units in the Illinois Basin. Efforts for this report have been mostly directed toward compilation of data for shale units. Miller et al. (1980) have reported results of triaxial and unconfined compressive tests and "Brazilian" indirect tensile strength tests on the New Albany Shale from cores taken along a NW-SE line across the Illinois Basin. Their data show a number of notable trends. Peak strengths and elastic moduli from unconfined compressive testing of samples loaded perpendicular to bedding ranged from 103 to 117 MPa and from 13,900 to 14,300 MPa, respectively. Samples loaded parallel to bedding showed higher unconfined compressive strengths (131 to 138 MPa) and higher moduli (23,900 to 29,900 MPa) than samples loaded perpendicular to bedding. Peak strength and modulus measurements for samples loaded parallel to bedding and subjected to a confining stress of 6.89 MPa (1000 psi) averaged 172 MPa and 9,860 MPa, respectively. "Brazilian" indirect tensile tests perpendicular to bedding showed an apparent

Table 2.4 Thermal conductivities of geologic units in the Illinois Basin.

Unit	Thermal Conductivity $\frac{BTU}{ft\ day\ ^oF}$	Thermal Conductivity $\frac{J}{m\ sec\ ^oC}$	Reference
glacial drift	4.3×10^{-7}	1.05	Cartwright, 1970
"Pennsylvanian rocks"	8.6×10^{-7}	2.09	Cartwright, 1970
"deep carbonate rocks"	1.2×10^{-6}	2.93	Cartwright, 1970
shales	6.9×10^{-7}	1.67	Heigold et al., 1971
limestone	9.0×10^{-7}	2.17	Heigold et al., 1971

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trend of increasing strength with distance toward the basin center and increasing depth of burial of the New Albany. Tensile strengths of samples from near surface in NW Illinois averaged 2.66 MPa. Samples from 300 m depths averaged 3.42 MPa, and samples from depths approaching 1000 m in central Illinois averaged 6.45 MPa.

2.2.4 *General Hydrologic Conditions and Setting*

The Illinois Basin probably contains a deep slow-moving ground-water flow system; however, data available at present do not adequately characterize that flow system for purposes of modeling. Few valid hydraulic head measurements have been documented in the large area of the basin, and movement of ground water in the basin is quantified only by indirect means, by inference from ground-water chemistry, and from temperature studies (Meents et al., 1952; Bredehoeft et al., 1963; Clayton et al., 1966; Bergstrom, 1968; Cartwright, 1970; Heigold et al., 1971; Bond, 1972).

Figure 2.9 summarizes current knowledge of the flow system along a north-south cross section (Figure 2.6). Data on total dissolved solids in the ground water show a shallow fresh-water zone across most of the basin. Near the northern end of the section, a large plume of fresh water penetrates deep into the basin along the highly permeable Ancell Group, indicating downward flow and recharge of the deep ground-water system (Meents et al., 1952; Bergstrom, 1968). Data on deuterium content of basin waters (Clayton et al., 1966) indicate that even the very saline brines of the deep basin have a meteoric and not a connate origin, suggesting that recharge by meteoric waters has since the emergence of the region in the late Paleozoic flushed the entire system of connate water.

Recharge to the deep ground-water flow system probably occurs in the outcrop belt that surrounds the basin. The difference in hydraulic head between rocks in the recharge area and the water table in the topographically low center of the basin ranges from 30 m (100 ft) to about 152 m (500 ft). This low relief on the water table produces gradients estimated at about 2.8×10^{-4} (Bredehoeft et al., 1963). Ground-water flow in the basin probably passes principally through the Mt. Simon, Ancell, Chesterian, and basal Pennsylvanian sandstone aquifers to the center of the basin where flow is upward through the rock sequence and surface discharge occurs. Temperature studies in the central part of the basin have identified unusually high geothermal

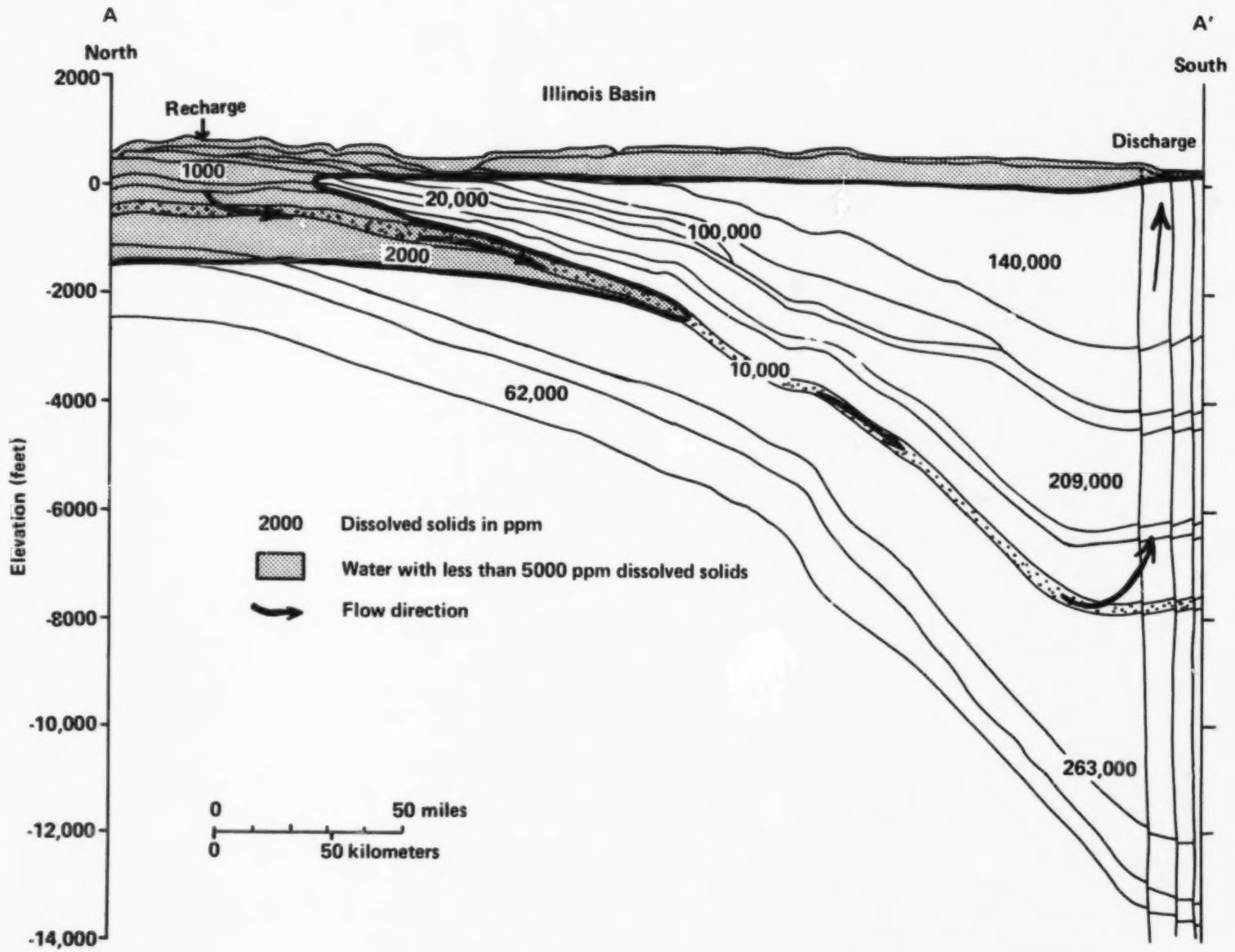

Figure 2.9 Generalized pattern of ground-water flow through the Illinois Basin. Location of cross section on Figure 2.5.

gradients that are probably associated with upward-flowing ground water (Cartwright, 1970; Heigold et al., 1971). These areas of upward flow generally coincide with structural features--i.e., the Wabash Valley Fault Zone and the DuQuoin Monocline (Figure 2.4), and it has been suggested that fluid is discharging upward through fracture zones associated with these features (Cartwright, 1970). In the area of the DuQuoin Monoclinal Belt, saline waters too brackish for human consumption immediately underlie the water table.

2.3 Williston Basin

2.3.1 *Location and General Geologic Setting*

The second region considered as a possible model for the RRS-SH is located on the southern flank of the Williston Basin in central South Dakota. This area contains a groundwater flow system that has been studied for nearly 100 years and has been cited as a classic artesian system. Extensive drilling to exploit water resources in confined high pressure sandstone aquifers and compilations of water level data for thousands of water wells provide an excellent data base for study of the hydraulic heads in the flow system. Data compiled during the first decade of this century before major drawdown of aquifer water levels identify a flow system at or near natural equilibrium, and comparisons of later measurements to early ones allows statements about the potential magnitude of the human influence on such a flow system. A second major attraction of the area for consideration as a candidate for the RRS-SH is occurrence of some of the thickest shale deposits in North America.

The area in which our efforts have been concentrated extends eastward from the Black Hills of southwestern South Dakota across the state to the broad lowlands of the James River basin. After detailed study of the Pierre Shale in the northern Great Plains, the U.S. Geological Survey recommended extensive further study of the Pierre in this region of South Dakota, because of its potential as an isolation medium for radioactive waste (Shurr, 1977). The Missouri River crosses the central part of the region and separates the Great Plains Province to the west from the glaciated Central Lowlands Province to the east. Topographic relief is sharp to gently rolling, and elevations range from above 1524 m (5000 ft) in the Black Hills to about 305 m (1000 ft) along the Missouri and James Rivers in the southeastern part of South Dakota.

East of the Black Hills a sequence of up to 1829 m (6000 ft) of Paleozoic to Cenozoic sedimentary rocks fills a southward extension of the Williston Basin. The geologic units are both continental and marine in origin and consist of carbonates, evaporites, sandstones, and shales. They overlie a complex of Precambrian igneous and metamorphic rocks consisting mainly of granite, quartzite, schist, and slate. During Late Cretaceous time the sedimentary sequence was deformed as the elongate dome of the Black Hills was uplifted. Post-Cretaceous erosion of the dome has truncated most of the sedimentary units, exposing Precambrian rocks in the center of the Black Hills. Truncated sedimentary strata now outcrop in concentric bands around the margin of the dome. It is in the high elevations of this outcrop belt that the principal sandstone and carbonate aquifers are recharged by precipitation and stream loss.

2.3.2 *Configuration of Geologic Units and Features*

The geologic map of South Dakota (Figure 2.10) shows the distribution of the principal geologic units in the state. Of particular importance to this study are (1) the concentric bands of the Black Hills outcrop belt, (2) the extensive outcrop area of the Upper Cretaceous shales and chalks east of the Black Hills, and (3) the extent of glacial deposits east of the Missouri River.

The stratigraphy of geologic units in central South Dakota is known both from studies of the Black Hills outcrops (Darton, 1909) and from studies of large numbers of well records in the rest of the state (Schoon, 1971). Table 2.5 presents a generalized stratigraphic column for central South Dakota. Geologic units in the sequence range in age from Precambrian to Quaternary and include a wide variety of rock types. Like the Illinois Basin, the lower part of the Williston Basin contains Cambrian sandstones which are overlain by a thick sequence of Paleozoic limestones and dolomites. But, unlike the Illinois Basin, the upper part of the sequence is dominated by very thick shales.

A structure map of the top of the Greenhorn Formation (Figure 2.11) shows the eastward dip of the Greenhorn east of the Black Hills and the trough of the Lemmon Syncline with its axis oriented northwest toward the center of the Williston Basin. Units above and below the Greenhorn have the same general structural trends. Figure 2.12 shows in diagrammatic cross section the distribution of major units along a line from Rapid City in the Black Hills through the city of Pierre on the Missouri River to the James River. The thick Upper Cretaceous shales (Pierre, Carlile, Belle Fourche, and Mowry Shales) clearly dominate the upper part

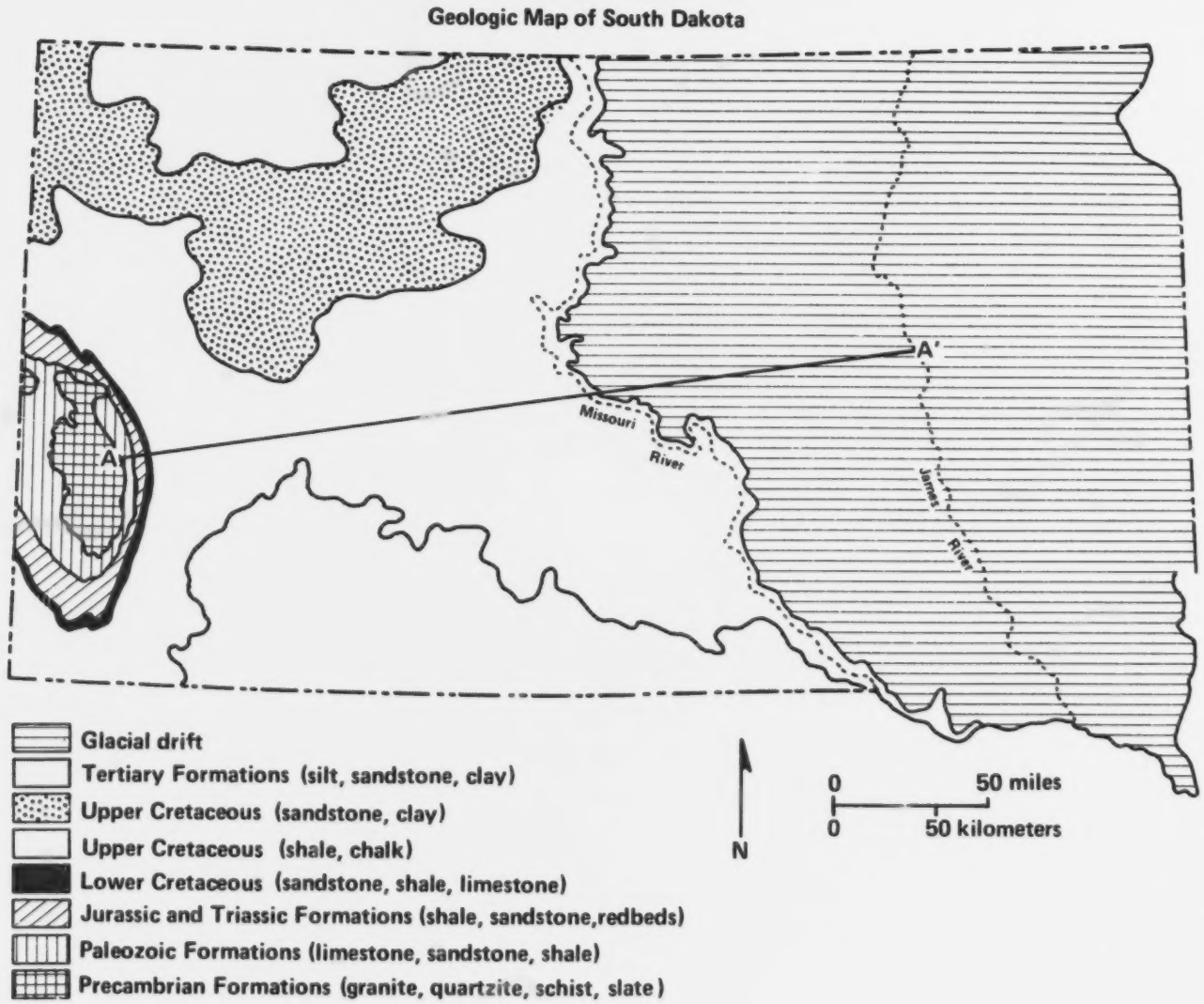

Figure 2.10 Map showing geology of South Dakota.

Table 2.5 Generalized geologic column for the southern flank of the Williston Basin.

Unit	Age	Dominant rock type	Thickness range (ft)
16. glacial drift	Quaternary	till, sand	0 - 500
15. Fox Hills Formation	Upper Cretaceous	sandstone	0 - 100
14. Pierre Shale	Upper Cretaceous	shale	0 - 1700
13. Niobrara marl	Upper Cretaceous	marl	100 - 200
12. Carlile Shale	Upper Cretaceous	shale	300 - 500
11. Greenhorn Formation	Upper Cretaceous	limestone	100 - 200
10. Belle Fourche to Mowry Formations	Upper Cretaceous	shale	200 - 400
9. Dakota Group	Lower Cretaceous	sandstone	200 - 500
8. Skull Creek Shale	Lower Cretaceous	shale	0 - 200
7. Inyan Kara Group	Lower Cretaceous	sandstone	200 - 300
6. Sundance and Morrison Formations	Triassic and Jurassic	shale, sandstone	0 - 500
5. Minnelusa Group	Pennsylvanian and Permian	limestone, dolomite evaporites, shale	0 - 1000
4. Madison Group	Mississippian	limestone	0 - 500
3. Red River to Duperow Formation	Ordovician to Devonian	limestone, dolomite	0 - 400
2. Deadwood Formation	Cambrian	sandstone	0 - 200
1. Precambrian basement	Precambrian	granite, quartzite	-

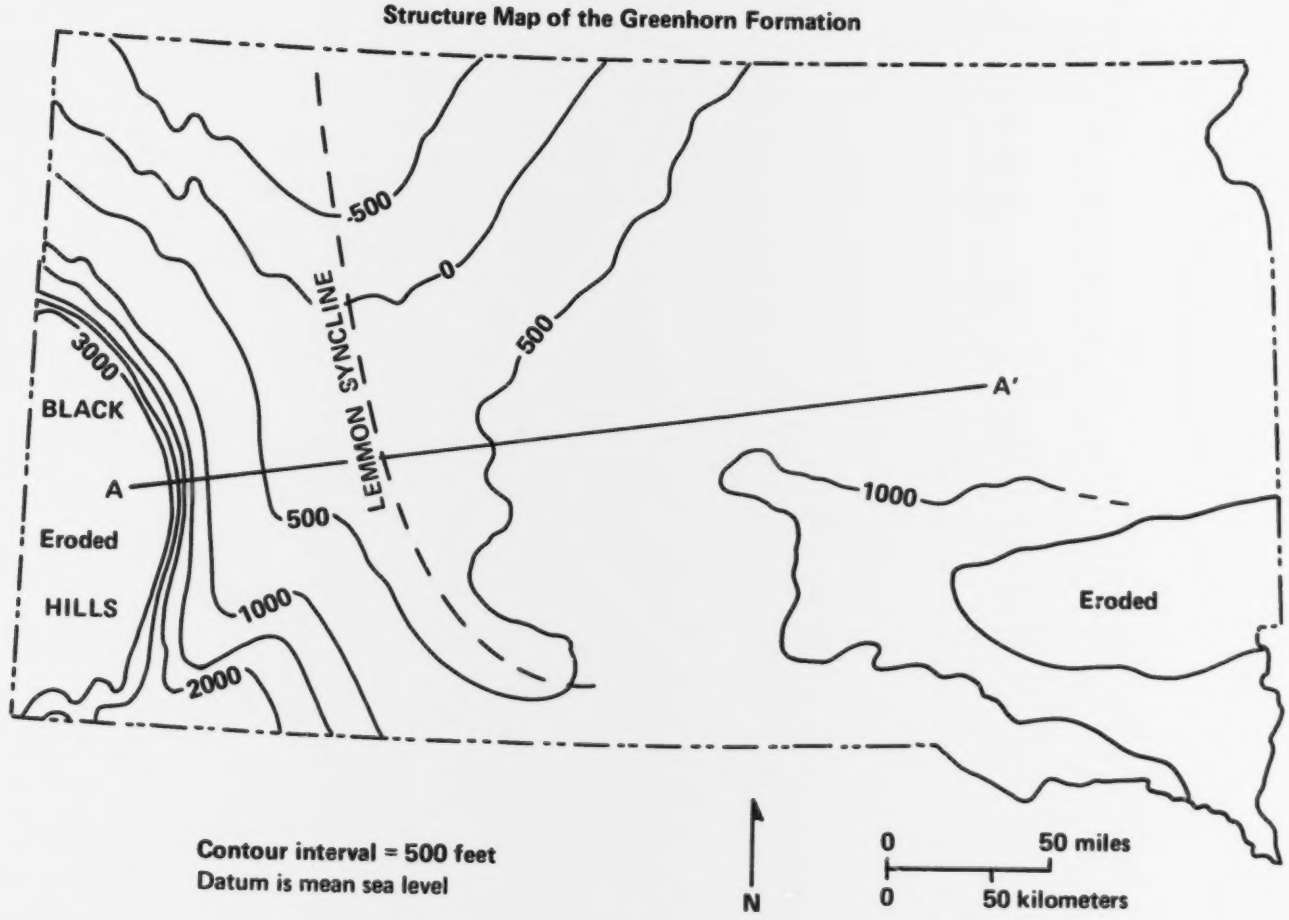

Figure 2.11 Map of structure on top of the Greenhorn Formation in South Dakota (after Schoon, 1971).

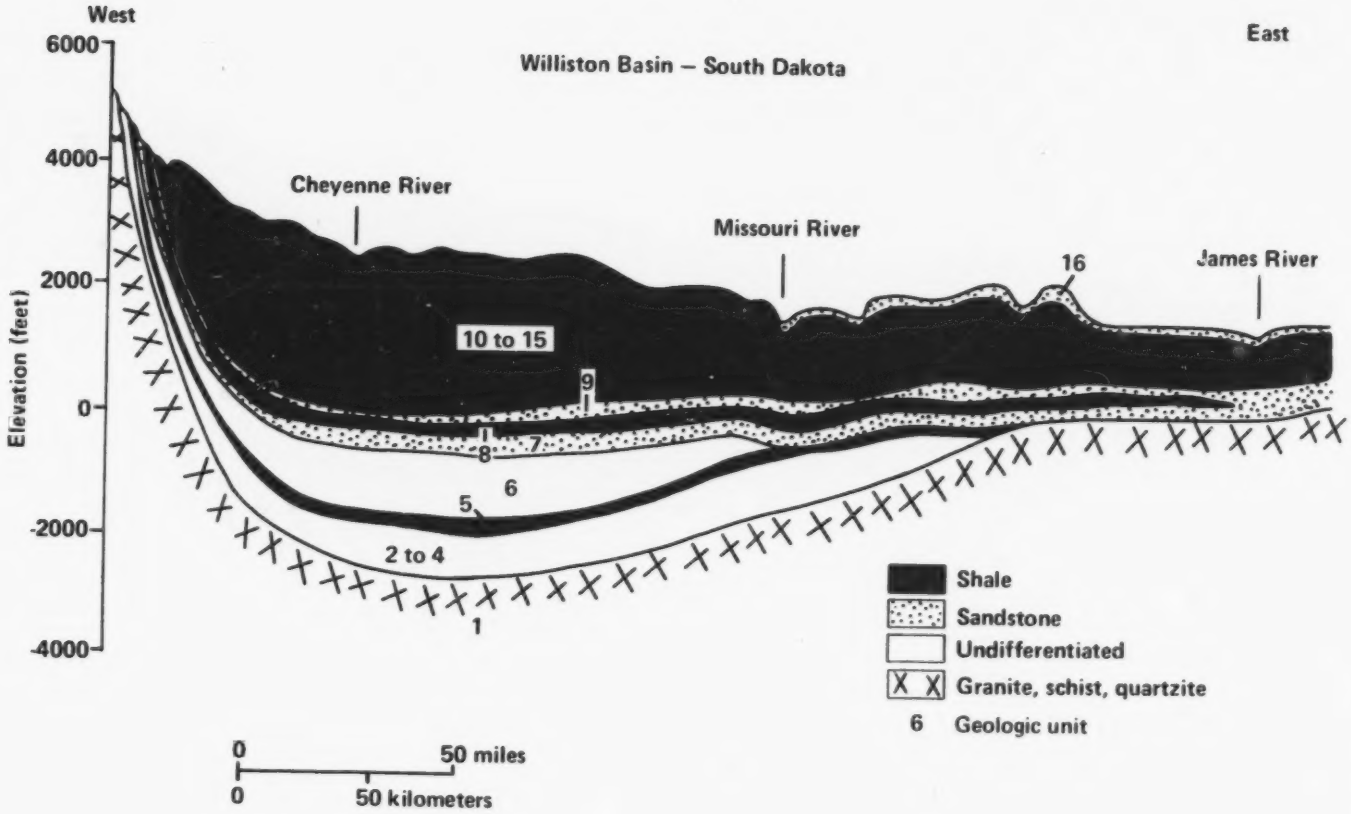

Figure 2.12 Diagrammatic cross section of southern flank of Williston Basin in South Dakota, showing principal geologic units listed in Table 5. Location of section shown on Figures 2.10 and 2.11.

of the sequence. Much of the apparent thinning of units near the Black Hills in Figure 2.12 reflects the vertical exaggeration of the cross section. Across most of the region the shales are gently folded; however, the dip of the bedding never exceeds a few degrees. No major faults are found in the Pierre, but some minor faulting with small displacements has been detected (Crandell, 1958).

Abel and Gentry (1976) report joints in each of the members of the Pierre in several near-surface excavations. All joints reportedly dip steeply, generally in excess of 60°. Joint frequency decreases with depth, but there is no information on either frequency or orientation at repository depths.

The Pierre Shale and the several Upper Cretaceous shales which underlie it would be the host units in a reference repository based on the Williston Basin. The Pierre has been the subject of a number of stratigraphic studies (Searight, 1937; Gries, 1942, 1954; Crandell, 1950). In some areas the Pierre Shale exceeds 610 m (2000 ft) in thickness and has eight named members distinguished on the basis of color, lithology, and carbonate content. These units consist mostly of light gray to black silty shale with limestone and ironstone concretions and many thin bentonite beds. The thin lowermost member of the formation is markedly different from the others and contains abundant organic matter. A detailed discussion of the lithology of units underlying the Upper Cretaceous shales in the Williston Basin probably has little relevance to this report and is not included for that reason.

2.3.3 *Properties of Geologic Units*

Because the Pierre Shale is stratigraphically equivalent to some of the Upper Cretaceous shales of the western Canada sedimentary basin, and because the Pierre has mineralogic and lithologic similarity to those shales, a detailed discussion of the properties of the Pierre will be largely applicable to the units chosen as host rocks for the RRS-SH. Compilations of most of the information available on properties of the Pierre have been made by Dames and Moore (1978) and Abel and Gentry (1975). The following discussion is based on these reports and supplemented by some more recent data.

2.3.3.1 *Hydrologic Properties* - The thick sequence of claystone, shale, bentonitic mudstone, and thin seams of bentonite that comprises the Pierre is largely devoid of aquifers and, although highly porous locally, is so impervious that it does not generally yield water to wells. Kemper

(1961) reported for the Pierre a very low hydraulic conductivity, 1.1×10^{-10} cm/sec (3.1×10^{-7} ft/day), and a relatively low porosity, 21 percent. However, Kemper used remolded samples for these measurements, and the values should not be considered representative of the natural material. Abel and Gentry (1975) report a range of conductivity for the Pierre of 1×10^{-6} to 1×10^{-10} cm/sec (2.8×10^{-3} to 2.8×10^{-7} ft/day) and a ratio of vertical to horizontal conductivity of from 0.5 to 0.1 because of the anisotropic nature of the shale. Average vertical and horizontal hydraulic conductivities suggested by Dames and Moore (1978) for intact Pierre Shale in the Williston Basin are 4.8×10^{-9} and 9.6×10^{-9} cm/sec (1.4×10^{-5} and 2.8×10^{-5} ft/day), respectively (Table 2.6). Porosity and natural moisture content are typically higher near the ground surface and decrease to relatively constant values (33 percent and 18 percent, respectively) below depths of 60 to 90 m. Rubey (1930) demonstrated that porosity decreased with an increase in the dip of Cretaceous shale beds in the Black Hills region and suggested that structural deformation causes a reduction in porosity. Rubey found the average porosity, average grain density, and bulk density of nine samples to be 29.5 percent, 2.66, and 1.88, respectively. For these samples, porosity ranged from 23.8 to 37.6 percent, average grain density ranged from 2.4 to 2.8, and bulk density ranged from 1.5 to 2.0.

Data on properties of other geologic units necessary for characterization of the entire natural system are sparse. This is primarily because the routine testing which has been performed as part of oil reservoir characterization in the other basins studied has not normally been performed for aquifer evaluations in the Williston Basin of South Dakota.

Sandstones included in the Dakota Formation and Inyan Kara Group are the principal aquifers in central South Dakota. Pumping tests conducted for a municipal water supply at Wall, South Dakota (Gries et al., 1976) indicate that these sandstone aquifers have hydraulic conductivities comparable to the most conductive sandstones of the Illinois Basin. Measurements averaged 5.0×10^{-4} cm/sec (1.42 ft/day). A number of limestone units beneath the Dakota, including those in the Madison and Minnelusa Groups, probably have high conductivities and serve as major water-conducting zones across the region from the Black Hills to the Missouri River. However, no data are available for the hydrologic properties of these units, or for most of the other units beneath them.

Table 2.6 Summary of properties of intact samples of Pierre Shale and associated Upper Cretaceous Shales

Tape of Property	Parameter	Mean (Range)	Reference
Index	Bulk Density	2.15	a
		1.88 (1.5 to 2.0)	b
	Average Grain Density	2.66 (2.4 to 2.8)	b
	Natural Moisture Content	27% <90m depth	c
		18% >90m depth	c
		(18 to 38%)all samples	c
	Porosity	33%	a
		29.5% (23.8 to 37.6%)	b
Hydrologic	Hydraulic Conductivity	(10^{-6} to 10^{-10} cm/sec)	c
	horizontal	9.6×10^{-9} cm/sec	a
	vertical	4.8×10^{-9} cm/sec	a
Thermal	Coeff. of Linear Thermal Expansion	No Data	
	Heat Capacity	No Data	
	Thermal Conductivity	No Data	
Mechanical	Young's Modulus	965 MPa	a
	Poisson's Ratio	0.2	a
	Bulk Modulus	536 MPa	a
	Shear Modulus	402 MPa	a
	Cohesion	(0.1 to 1.42 MPa)	a,c
	Friction Angle	(4 to 23)	a,c
	Compressive Strength		
	Peak at σ_3 = 5.5 MPa	10.0 MPa	d
	Peak at σ_3 = 2.8 MPa	6.2 MPa	d
	Residual at σ_3 = 5.5 MPa	9.3 MPa	d
	Residual at σ_3 = 2.8 MPa	5.9 MPa	d
	Tensile Strength	0.34 MPa	a

a Dames and Moore, 1978
b Rubey, 1930 (mostly near-surface samples)
c Abel and Gentry, 1975
d Kim and Ko, 1977

2.3.3.2 *Geochemical Properties* - The Pierre Shale in the northern Great Plains has been classified as a "soil like" clay shale (Abel and Gentry, 1975), because it normally contains more than 50 percent clay-size particles and lacks any significant quantity of intergranular cement. Tourtelot (1962) determined from size analyses on 38 samples that the Pierre contains an average of 70 percent clay (sizes smaller than 4 μm) and the clay content ranges from 35 to 90 percent. Smaller than 1 μm size clay comprises 50 percent of the shale in places. In central South Dakota, the Pierre averages 75 percent smaller than 4 μm clay.

Most of the Pierre Shale from the region between the Black Hills and the Missouri River consists of 65 to 80 percent clay minerals, 15 to 25 percent quartz, a few percent feldspar, and small amounts of calcite, dolomite, biotite, pyrite, gypsum, jarosite, and organic matter. The clay minerals consist of 25 to 45 percent smectite, 35 to 45 percent mixed-layer illite-smectite, 15 to 25 percent illite, and about 5 percent kaolinite and 5 percent chlorite (Tourtelot et al., 1960).

Trace element analysis of Pierre shale samples from the northern Great Plains are discussed by Tourtelot et al. (1960). Of particular interest in the present report are U and Sr contents, which are reported to range from 3 to 12 and 115 to 620 ppm (parts per million), respectively.

2.3.3.3 *Thermal Properties* - Information on thermal properties of the Pierre Shale is conspicuously absent from Table 2.6. No specific data are available on the effects of high temperature on the structural stability of the shale. Some recent laboratory experiments (Lappin and Olsson, in press) have suggested that a sample of Pierre Shale containing 75 percent clay, of which 75 percent is mixed-layer illite-smectite containing 60 percent smectite interlayers, should undergo 2.2 ± 0.3 percent linear contraction upon heating to 100°C. This effect is produced by a dehydration of smectite and occurs in a temperature range through which most other rock types exhibit a thermal expansion.

The geothermal gradient has been mapped in South Dakota by Schoon and McGregor (1974). Their data show a gradient in the region between the Black Hills and the Missouri River that varies from about 17°C/km to over 100°C/km. Most of the region has a gradient of about 34°C/km. The highest gradients occur in a narrow zone along the Missouri River and probably result from marked upward flow of deep ground water in that region.

2.3.3.4 *Mechanical Properties* - Values of various parameters used to characterize the mechanical behavior of intact Pierre Shale are compiled in Table 2.6. The values shown here indicate that the Pierre is much weaker than most shales. The cohesion and angle of internal friction of the Pierre reported by Dames and Moore (1978) range from 0.01 to 0.21 MPa (2 to 30 psi) and 8 to 25 degrees, respectively, as compared to 2.76 to 29.6 MPa (400 to 4300 psi) and 15 to 33 degrees for a typical shale. Strength tests on samples of Pierre Shale conducted by Kim and Ko (1977) at confining pressures up to 5.52 MPa (800 psi) and peak strengths up to 10.3 MPa (1500 psi) indicate the following apparent cohesion and internal friction angles:

	Cohesion	Friction Angle
Single Stage Triaxial Testing	1.42 MPa (206 psi)	5.3°
Multi-Stage Triaxial Testing	1.41 MPa (204 psi)	4.2°

Peak and residual strengths of Pierre Shale measured at various confining pressures are shown in Figures 2.13 and 2.14.

The low strength, high porosity, and high smectite composition of the Pierre Shale support observations by Schultz (1978) that the maximum depth of burial of the Pierre in central South Dakota was never more than about 300 to 600 m. Mechanical properties of the Pierre also indicate that it is much weaker than the illitic New Albany Shale of the Illinois Basin. The Young's modulus, unconfined strength and tensile strength of the New Albany are all an order of magnitude or more higher than those for the Pierre.

2.3.4 *General Hydrologic Conditions and Setting*

Early concepts of the workings of the artesian ground-water system east of the Black Hills held that meteoric waters recharged the Lower Cretaceous Dakota Sandstone at outcrops in the Black Hills, were transported through the Dakota aquifer system to eastern South Dakota, and discharged through outcrops (Shepard, 1895; Darton, 1909). These early models envisioned a single continuous sandstone body confined by shales and extending from recharge to discharge areas. Russell (1928) identified five substantial inconsistencies between observed field relations and the simple artesian model. He observed that (1) the sandstones of the Black Hills are older than the type Dakota in northeastern Nebraska, (2) continuity of sandstone units between the

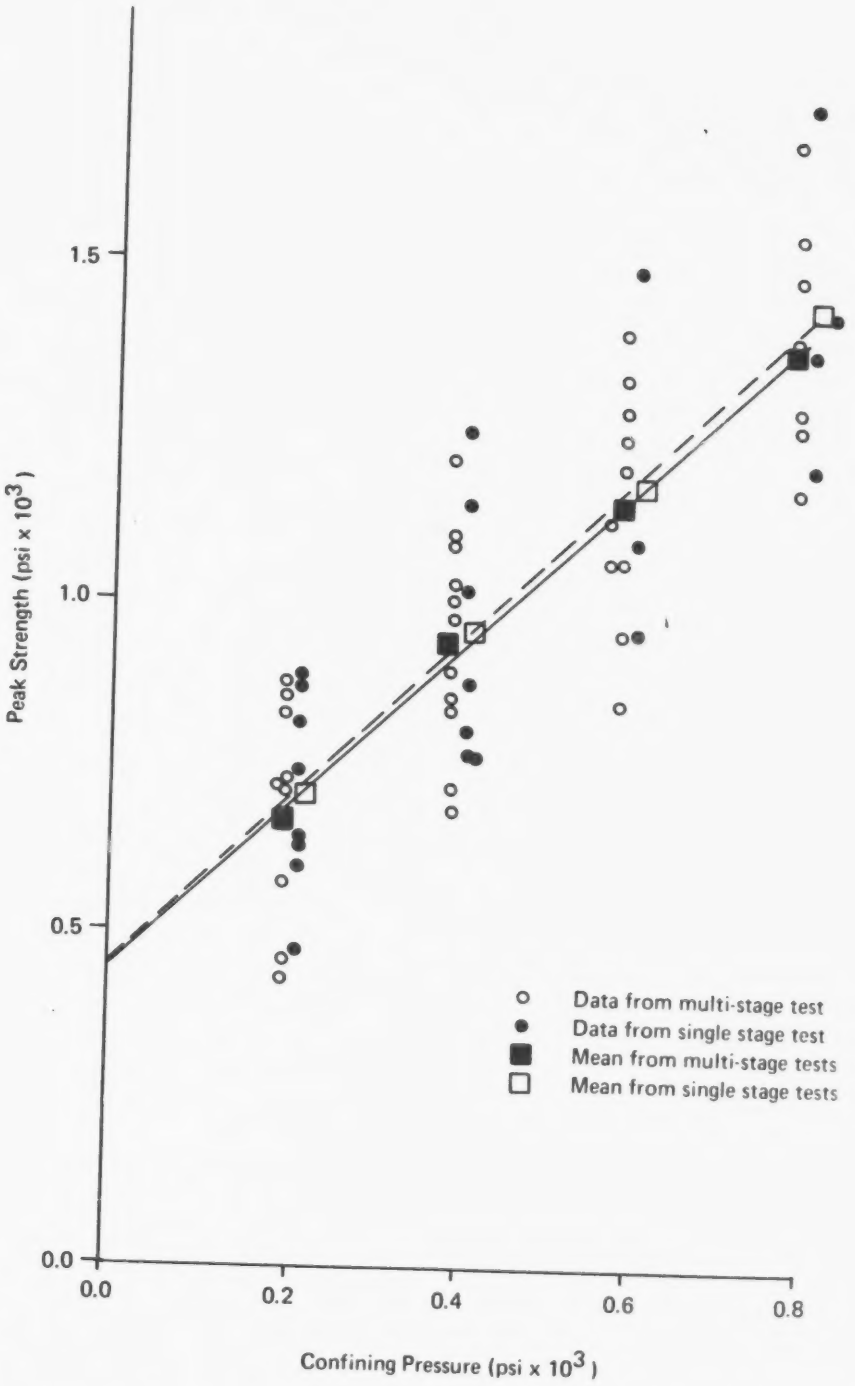

Figure 2.13 Peak strength of Pierre Shale samples at various confining pressures. Linear regression lines are shown for multi-stage (solid) and single stage (dashed) triaxial tests (after Kim and Ko, 1977 , in Dames and Moore, 1978). 145 = 1 MPa.

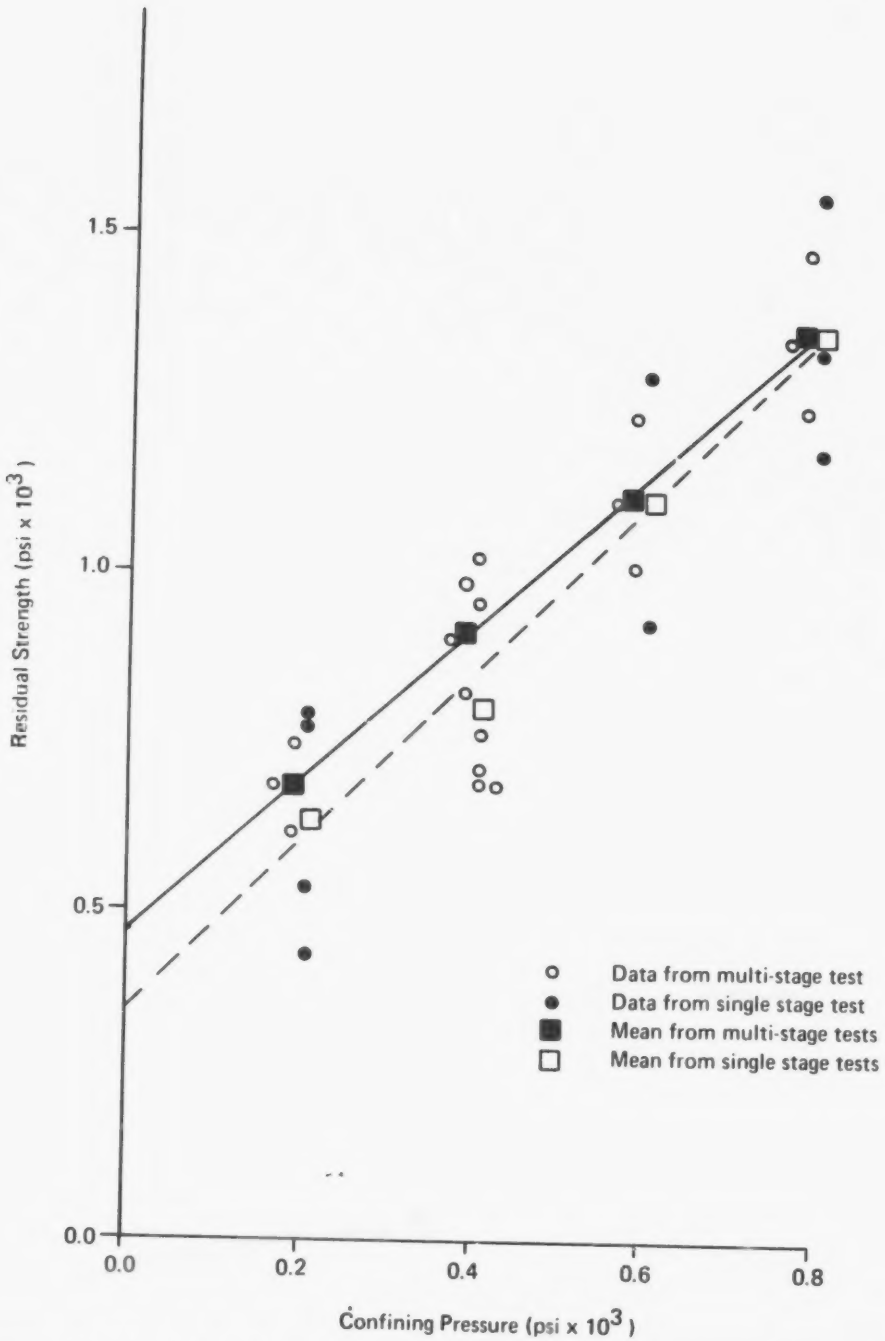

Figure 2.14 Residual strengths of Pierre Shale samples at various confining pressures. Linear regression lines are shown for multi-stage (solid) and single stage (dashed) triaxial tests (after Kim and Ko, 1977, in Dames and Moore, 1978). 145 = 1 MPa.

Black Hills and the type area had not been demonstrated, (3) the sandstone sequence in some regions is highly lenticular and contains large quantities of shale, (4) there exist differences in chemical quality and in pressure between waters of the "upper and lower parts" of the aquifer system, and (5) there are large lateral variations in chemical quality of the water in the system. As an alternative to the confined sandstone artesian model, Russell proposed an explanation involving sedimentary compaction to generate pressures in connate waters. This has subseqently been judged a less likely explanation. Although Russell's (1928) alternative was not accepted, his observations encouraged serious re-evaluation of existing hypotheses.

Largely through the stratigraphic studies of Gries (1954) it is now known that the thick sandstones of the type Dakota thin westward and intertongue with shales in the western third of South Dakota. Only the thin lowermost tongue, the Newcastle Sandstone, extends as far west as the Black Hills, and it crops out sporadically over a narrow belt. Because of the restricted outcrop area, the Dakota probably receives little direct recharge from precipitation or stream flow.

Recent studies have shown that the sandstones of the Inyan Kara Group, once believed to be part of the Dakota Group, crop out over a sizeable area in the Black Hills, are more uniform than the Dakota in their regional thickness, and over most of the western two thirds of South Dakota are stratigraphically and hydrologically separated from the Dakota by the Skull Creek Shale (Figures 2.12 and 2.15).

The existence of this separate sandstone body, the Inyan Kara Group, that can receive substantial recharge from meteoric waters and is separated from the Dakota by a thick shale, helps explain the occurrence of the different pressures and water compositions observed by Russell (1928) in the "upper and lower parts of the Dakota".

Detailed studies of older, pre-Cretaceous units in South Dakota have identified several additional aquifers below the Inyan Kara which, where intervening units are thin or absent, can recharge the Dakota from below. Swenson (1968) postulated that the principal sub-Dakota aquifer is the Madison Limestone (Mississippian), a cavernous limestone across which streams in the Black Hills lose a substantial quantity of their flow (Brown, 1944). Schoon (1971) has since proposed that several permeable zones within the interval between the top of the Inyan Kara and the top of the Roundtop Shale (Pennsylvanian Minnelusa Group) yield substantial quantities of water to the Dakota east of the Missouri River where the Skull Creek Shale is absent. In

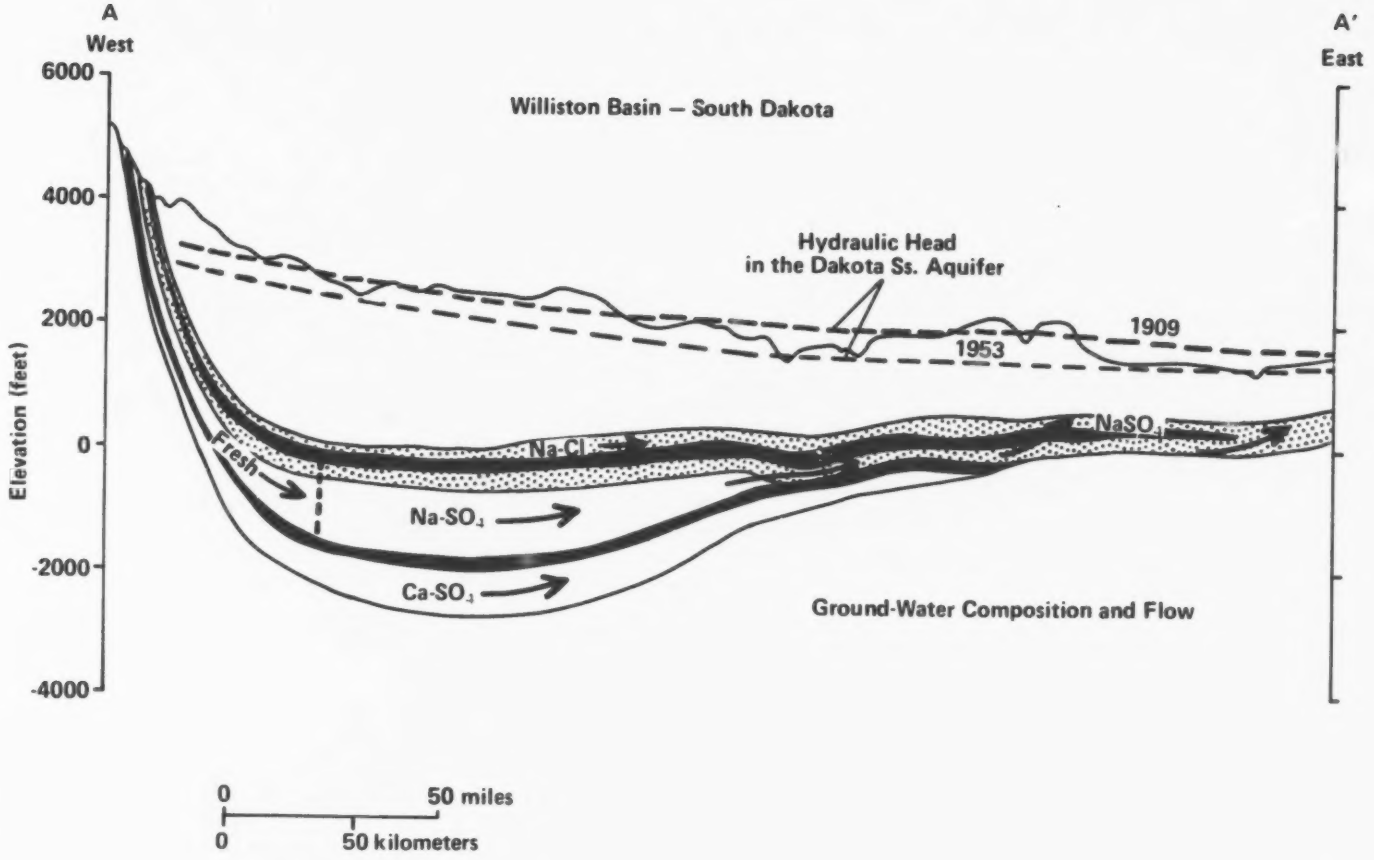

Figure 2.15 Generalized pattern of ground-water flow through southern flank of the Williston Basin in South Dakota. Location of section shown on Figures 2.10 and 2.11.

addition, the interval that includes the Madison Limestone and that extends from the base of the Roundtop Shale to the top of the Precambrian, yields water to the Dakota in southeastern South Dakota where both the Roundtop and Skull Creek Shales are absent.

Regional variations in water chemistry are easily understood when the pattern of recharge of the Dakota by underlying aquifers carrying waters of various compositions is known (Figure 2.15). In a large part of western South Dakota, where the Inyan Kara and subjacent aquifers are isolated from the Dakota by the Skull Creek Shale, the Dakota contains sodium-chloride type water, interpreted by Schoon (1971) to be connate water. In this same region the underlying Inyan Kara Group contains water that is fresh near the outcrop and gradually with distance along the flow path becomes a sodium-sulfate type water. East of the pinch out of the Skull Creek, the principal water type found in the Dakota is a sodium-sulfate type derived from the Inyan Kara to Roundtop interval. In southeastern South Dakota (not shown on Figure 2.15) where the Roundtop Shale is absent, calcium-sulfate waters from the Roundtop to Precambrian interval are the dominant type in the Dakota.

The flow system just described for the Lower Cretaceous sandstones of the Dakota Formation and Inyan Kara Group constitute a heavily pumped artesian water resource that today supplies the water needs of nearly 25 percent of the population of South Dakota. The first wells drilled to tap these aquifers were probably completed in the early 1880's, and by 1890 an estimated 100 or more successful wells were scattered through thirty or more counties (Culver, 1890). By 1909, more than 1000 wells had been developed in the "Dakota" sandstones east of the Missouri River (Darton, 1909). By 1922, the number topped 8000, and by 1970, about 15,500 wells had been drilled (Schoon, 1971). This heavy development, with annual withdrawals now exceeding 114 billion liters (30 billion gal), has caused widespread decline in hydraulic head. Head losses of nearly 122 m (400 ft) have been documented in some heavily pumped regions.

The history of pumpage and the large head losses experienced in this part of the Williston Basin serve to emphasize some points of concern in the modeling of reference repositories after natural systems. Many natural hydrologic systems are already highly perturbed by human action, and one should be cautious regarding the use of perturbed systems as a basis for a reference repository. We must take care to examine the magnitude of the potential human influence on ground-water flow. As an example, the water levels in the Dakota measured by Darton prior to 1909 (Figure 2.15) probably reflected a natural artesian system near the equilibrium state that existed prior to pumping. In 1909 across much of South Dakota, the hydraulic gradient across

the Pierre Shale was vertical, causing upward flow toward the ground surface. By 1953, pumping had lowered water levels to such an extent (Figure 2.15) that flow directions have probably been entirely reversed through large portions of the Pierre--i.e., flow is now downward through much of the Pierre Shale.

2.4 Western Canada Sedimentary Basin

2.4.1 *Location and General Geologic Setting*

The third candidate shale repository system that we have examined has been selected as the model for the RRS-SH. It is located in part of the western Canada sedimentary basin, north of the Alberta-Montana border. The study area comprises approximately 28,000 km^2 in the plains of southeastern Alberta (Figure 2.16) and extends from Township 1 to 15 North and from Range 1 to 20 West of the 4th Meridian. The area is semi-arid. Temperatures often range from $-37^{o}C$ to $+37^{o}C$ on an annual basis with a mean annual temperature of approximately $5^{o}C$. Although precipitation averages approximately 340 mm yearly, it varies from 160 to 475 mm. Of the total precipitation, approximately 65 percent falls as rain from April to September. Evapotranspiration is approximately 600 mm per year. The geology generally consists of an alternating sequence of thick, very low permeability shale units and thinner but more permeable sandstone units. Data are available to a depth of approximately 1800 m for many of the more permeable units because of the active programs of exploration for oil and gas in the region. The information upon which our studies are based comes from an evaluation of geological literature, unpublished geological and hydrogeological studies on file with various government agencies, and an original synthesis of the abundant primary data available for this area.

2.4.2 *Configuration of Geologic Units and Features*

The entire stratigraphic section for bedrock ranges in age from Precambrian to Tertiary. Figure 2.17 presents a generalized stratigraphic column for the study area. Because most of the existing data is available for rocks ranging in age from Mississippian to Cretaceous, we have studied this part of the sequence in greatest detail. Figure 2.18 is a three-dimensional fence diagram that shows the regional geology. The dominant lithology in this sequence of rocks is shale, with occasional sandstone units and minor amounts of coal and carbonates. Most units have

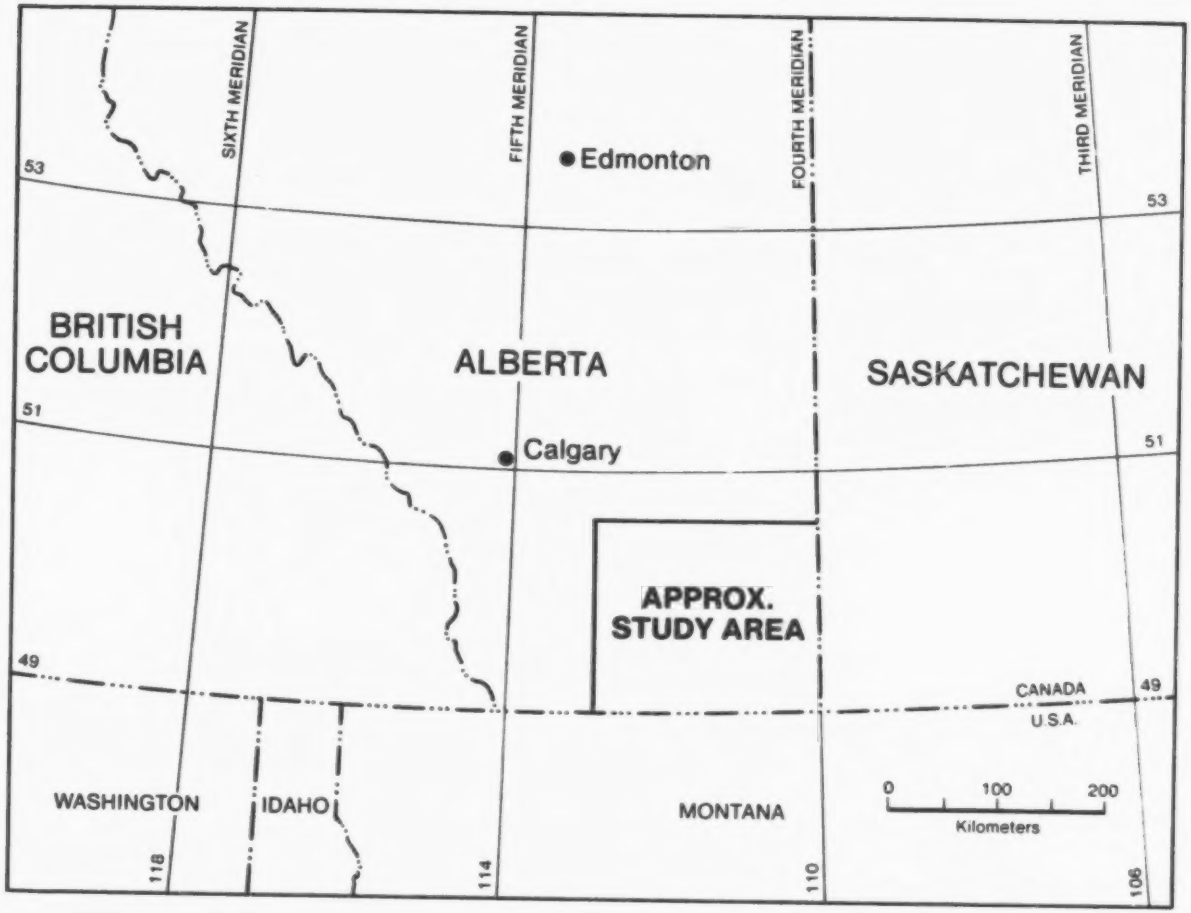

Figure 2.16 Map showing location of study area in southeastern Alberta, Canada.

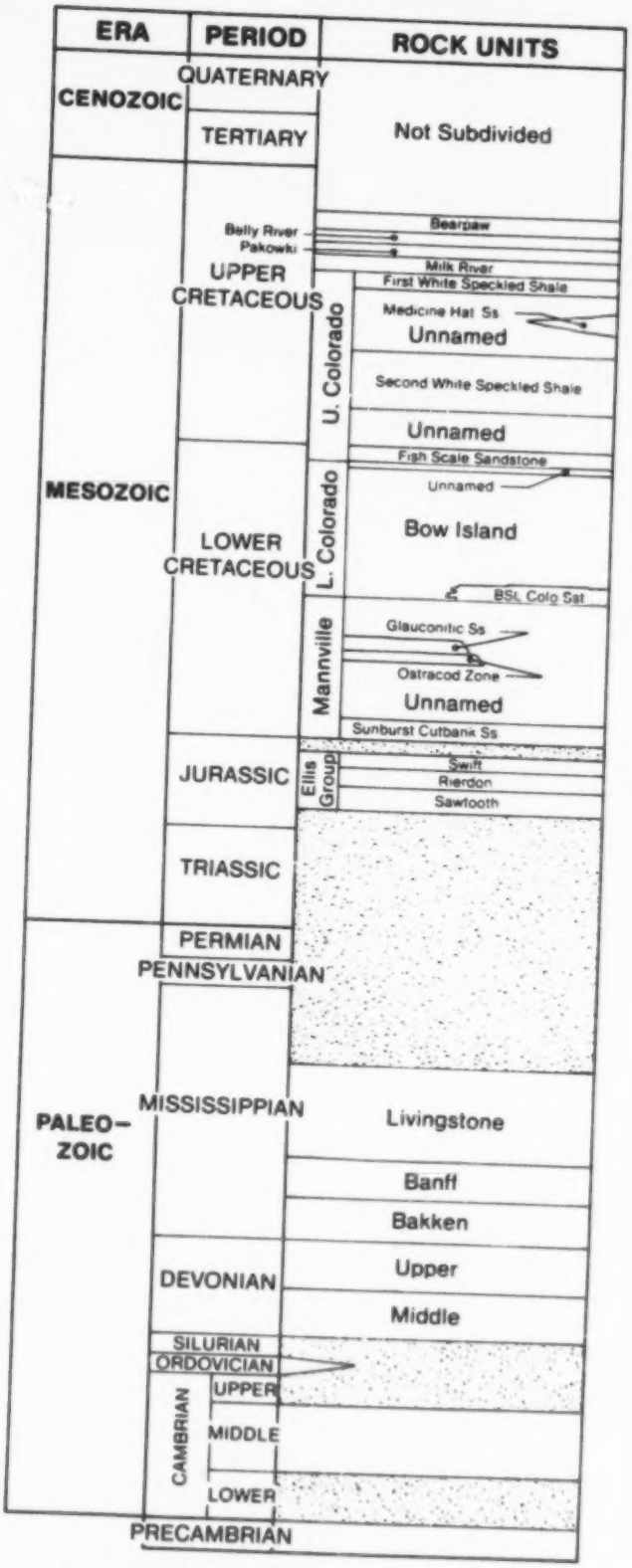

Figure 2.17 Generalized stratigraphic column for western Canada sedimentary basin. Shaded portions represent unconformities.

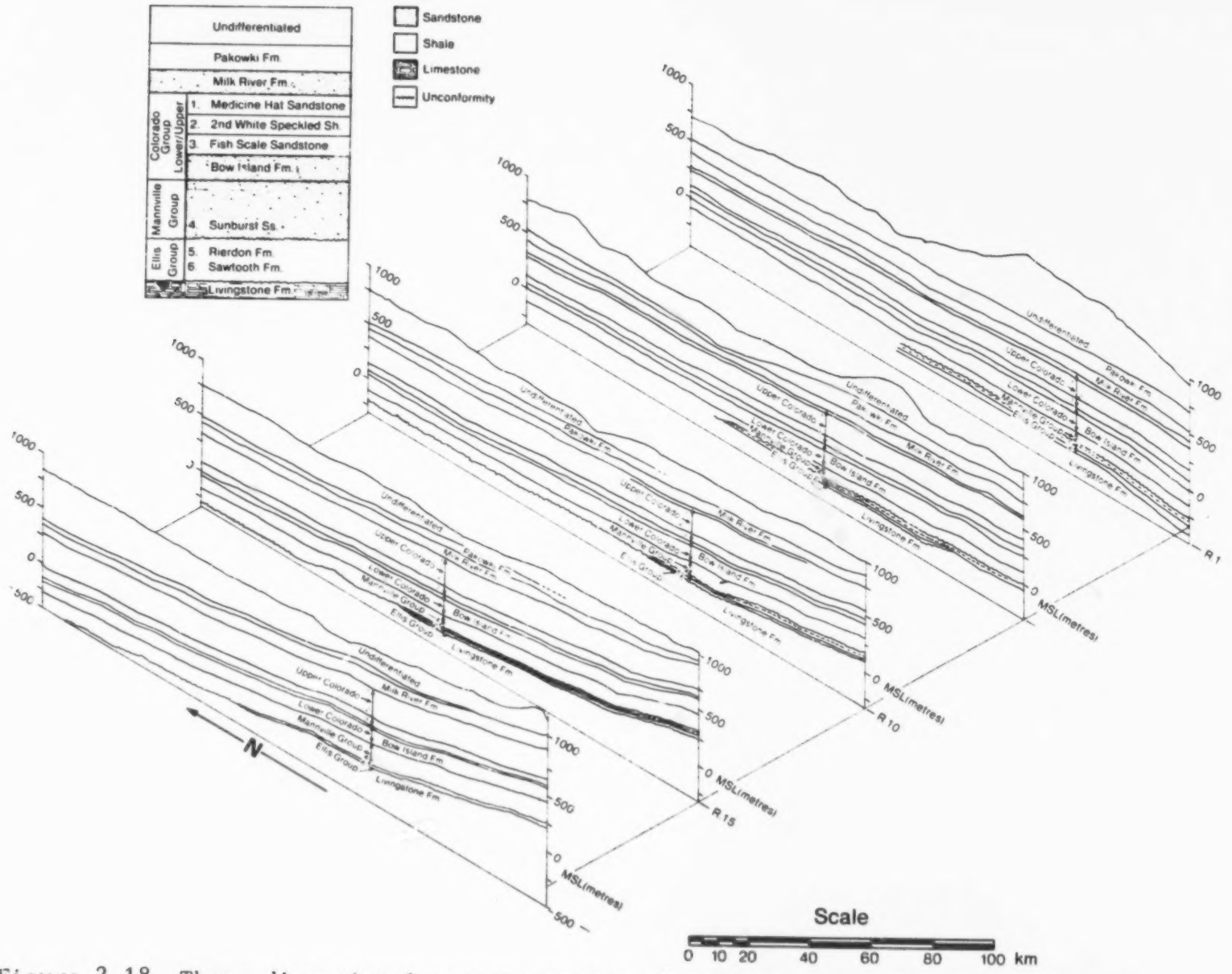

Figure 2.18 Three-dimensional representation of geology of southeastern Alberta.

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been tested and sampled using conventional oil-field methods. Several contain quantities of oil and gas. In order to depict the extent of shale units in the upper part of the section, a correlated cross section of electrical resistivity and self-potential (S.P.) logs has been prepared for a north-south line across the study area (Figure 2.19). Note the extensive thickness of shale in the upper part of the sequence shown by uniformly low resistivity and low S.P. curves.

2.4.2.1 *Geologic Structure* - The major structural feature in southeastern Alberta is the Sweetgrass Arch, a broad northward plunging anticlinorium with a history of movement dating back to Jurassic and Mississippian times (Tovell, 1958). This arch extends from Montana into Alberta and consists of three major tectonic elements and a series of subsidiary folds. The strata are gently dipping to the east, north, and west as shown in Figure 2.20. The fence diagram (Figure 2.18) shows these trends in vertical cross sections. The major tectonic elements in Alberta are the northward extension of the Kevin Sunburst dome and the northeast-plunging Bow Island arch. The structure contour map of the Milk River Sandstone (Figure 2.20) shows these features and a number of subsidiary folds superimposed on the major tectonic elements. The smaller features are generally northward- or eastward-plunging anticlines and synclines. There appears to be no significant faulting associated with these structures.

Recent studies of surface and subsurface fracture orientations in southern Alberta (Babcock, 1974; 1978) have identified two orthogonal joint systems made up of vertically dipping extensional fractures perpendicular to bedding. The first system has sets striking northeast and northwest, roughly parallel with and normal to the trend of the Rocky Mountain orogenic belt to the west. The set striking northeast is usually dominant in terms of being the set most commonly developed, and also because joints of this set are usually cross cutting, with joints of other sets terminating against them. The second orthogonal system has sets striking north-south and east-west (Babcock, 1978). The two joint systems are found in diverse rock types that range in age from Devonian to Paleocene. The patterns of joints show a remarkable similarity of strike over an area of many thousands of square kilometers and throughout a stratigraphic section of several thousand meters.

A detailed study has been made of joint azimuths measured at outcrops in a 6500 km^2 region just to the northwest of our study area (Babcock, 1978). In outcrop, joint sets are

Figure 2.19 North-south cross section of electric logs.

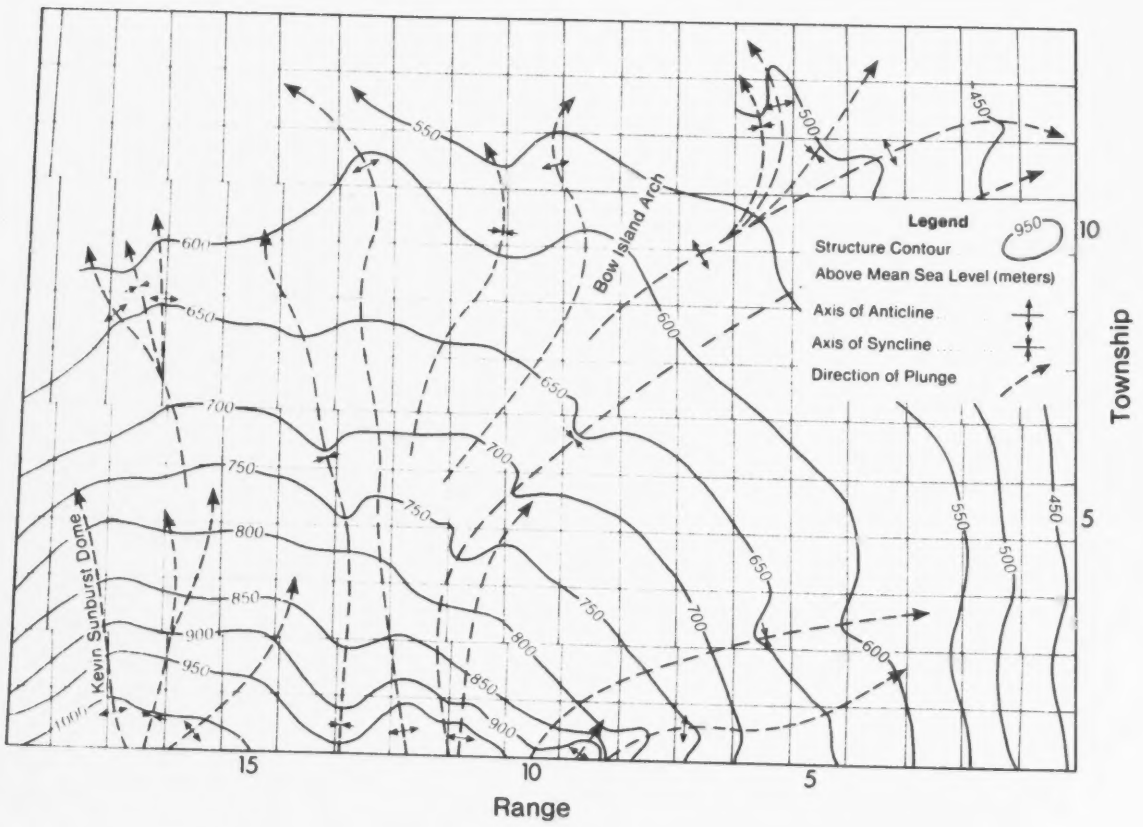

Figure 2.20 Map showing structure on top of Milk River Formation and local structural features in southeastern Alberta (after Meyboom, 1960).

well defined; sets striking slightly west of north, northwest, and northeast are the most prominently developed. The fractures of these regional systems are, in general, 10 to 100 m in length. Fractures in shale are more closely spaced (0.5 to 20 cm) than in associated sandstones (15 cm to 1 m) in surface exposures. There is no information on fracture aperture or on changes in aperture, spacing, or orientation with increasing depth. The principal fracture systems do not exhibit any change in strike across the Sweetgrass Arch, indicating they formed independently of this flexure.

Based on the tectonic setting of the region and discussions with engineers involved with hydraulic fracturing, Babcock (1978) suggested that the intermediate principal stress in the southern Alberta plains is normal to the trend of the Rocky Mountain orogenic belt, or roughly northeast-southwest. The maximum stress is vertical, and the minimum stress direction is inferred to be northwest-southeast, parallel with the trend of the Rocky Mountains. Neither the orientation nor magnitude of stresses have been measured in the field. Some reorientation of stresses in the area of the Sweetgrass Arch might be expected because of the different geometry of deformation there as compared with much of western Alberta along the Rocky Mountain orogenic belt.

The geologic map of southeastern Alberta (Figure 2.21) shows an outcrop pattern controlled by the Sweetgrass Arch. The oldest rock units are found in the south-central portion of the region, with younger units occurring on the flanks of the structure to the east and west.

2.4.2.2 *Description of Geologic Units* - The Precambrian basement underlying the study area consists of coarse plutonic igneous and metamorphic rocks. These rocks are unconformably overlain by Cambrian sediments consisting of a basal conglomeratic sandstone, followed by interbedded shale and calcareous silt, and fine grained sandstone (Webb, 1951). Limestone becomes more prominent westward in the study area. The Cambrian units, as a whole, become thinner eastward.

Pre-Devonian erosion removed Silurian, Ordovician, and Upper Cambrian rocks from much of the study area. Only a thin wedge of Ordovician rock is preserved in southeastern Alberta where it is comprised largely of dense brown microgranular dolomite (ASPG, 1966). Over most of the study area, Middle Devonian rocks rest unconformably on Middle Cambrian rocks. The Middle Devonian is composed of a cyclical sequence of carbonate and evaporite units with thin clastic beds. Westward from the study area, increasing

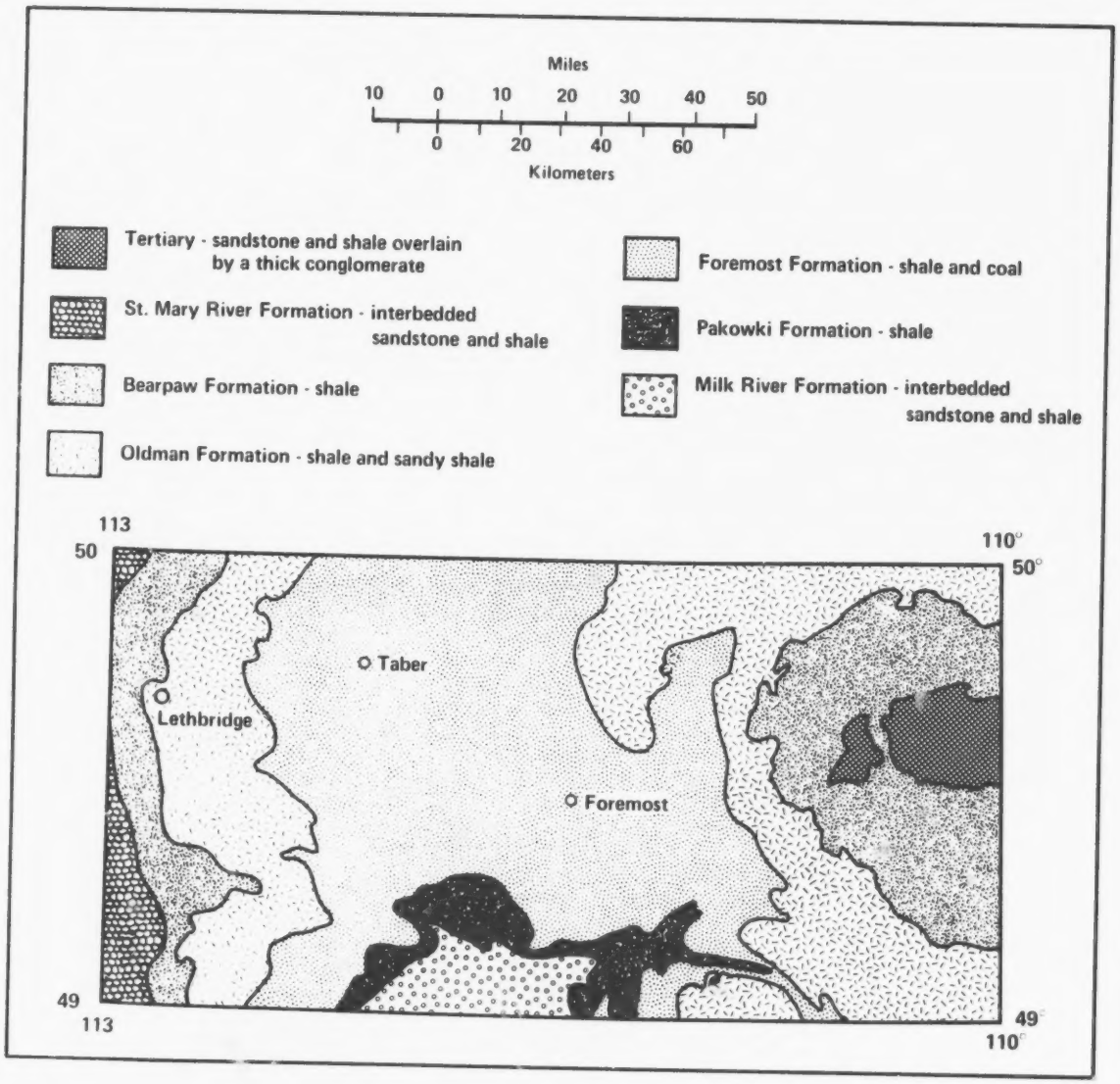

Figure 2.21 Map showing bedrock geology of southeastern Alberta (after Meyboom, 1960).

amounts of anhydrite are encountered. The Upper Devonian consists of a sequence of shale, shaly limestone, argillaceous dolomite and limestone, anhydrite, and siltstone (ASPG, 1966).

Mississippian sedimentation was continuous from the Upper Devonian. Mississippian rock units in the study area consist of, in ascending order, the Bakken, Banff, and Livingstone Formations. The Bakken Formation is divided into four lithologic units: black shale at the base and top of the formation, a medial sand, and at many locations a dolomitic siltstone overlying the basal shale (Penner, 1958). The sandstone unit is light gray, fine grained, quartzose, and slightly calcareous. The Bakken Formation diminishes in thickness towards the east where it is only recognizable as a thin black shale bed (Penner, 1958).

The lower part of the Banff Formation consists of a dark brown and gray, argillaceous, cherty limestone and calcareous shale. The lithology of the upper part of the Banff Formation is highly variable. The rock types are fine grained, arenaceous and slightly argillaceous limestone, shale, dolomitic siltstone to sandstone, finely crystalline, sparsely crinoidal limestone and minor amounts of interbedded coarse crinoidal limestone.

The Livingstone Formation is a massive gray-weathering medium to coarse crystalline crinoidal and fragmental limestone. It has been partly altered to dolomite and interbedded with argillaceous, arenaceous, and cherty limestone and dolomite (ASPG, 1966). Northwest of the study area, the Livingstone equivalent includes the Pekisko, Shunda, and Turner Valley Formations. Figure 2.22 shows structural contours on the top of the Mississippian.

Unconformably overlying the Mississippian formations is the Ellis group of Jurassic age which in the study area consists in ascending order of the Sawtooth, Rierdon, and Swift Formations. The Sawtooth Formation directly overlies the Mississippian limestone over most of the study area. Irregularities in the Mississippian limestone surface influence the thickness and extent of the Sawtooth Formation (Figure 2.23). The top of the formation consists of a green shaly sand or sandy shale with scattered chert pebbles and distinctive fossils. Beneath this bed is a quartz sandstone varying in thickness from 0.5 to 10 m. This unit is a white quartz sandstone, fine to medium grained and well sorted. Locally it may be shaly or cemented by calcite. Underlying this sandstone is a dark green and noncalcareous shale. In the eastern part of the study area, this shale appears to interfinger with oolitic limestone and the subdivision of the formation is difficult (Wier, 1949).

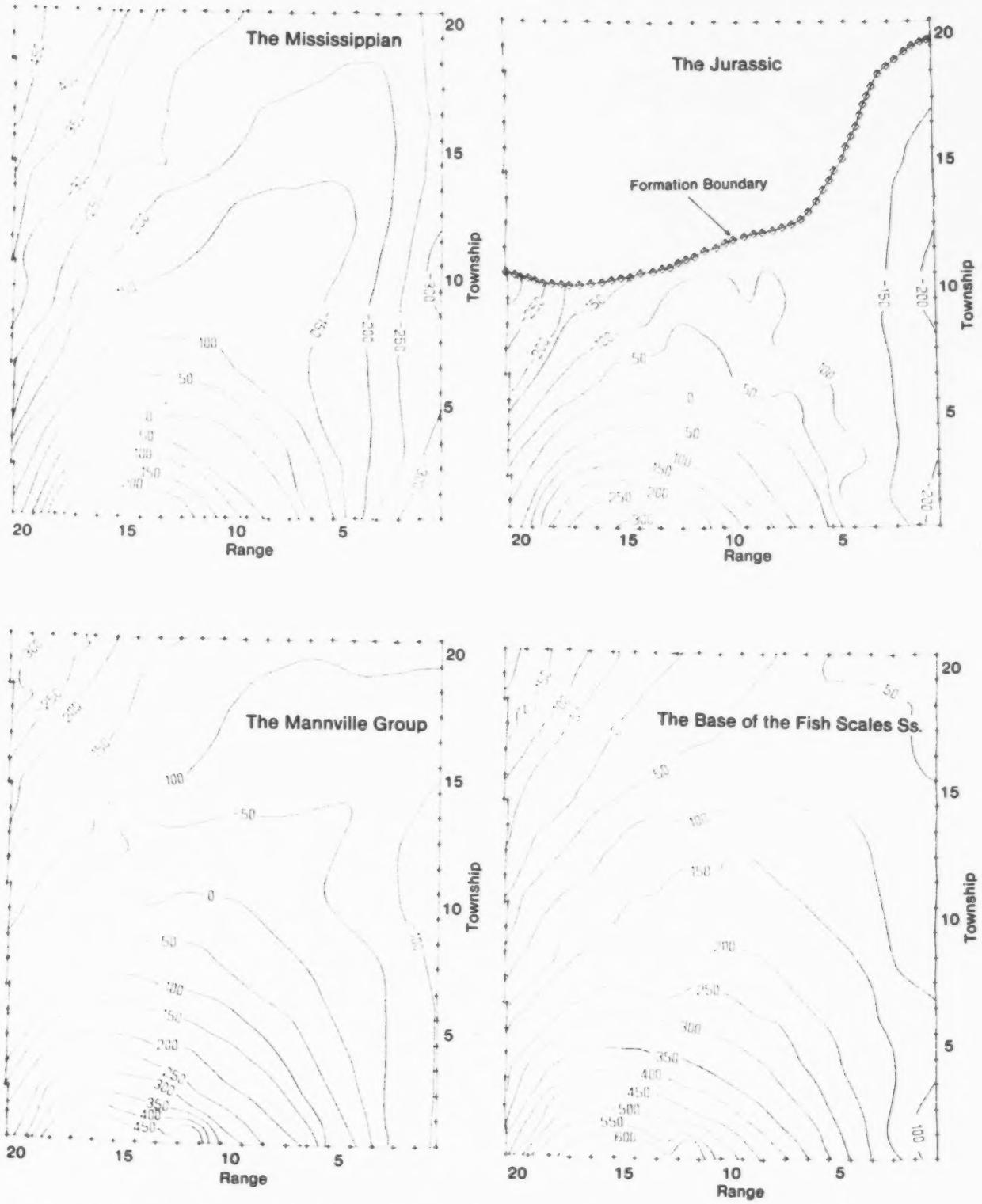

Figure 2.22 Maps showing structure of geologic units in south-eastern Alberta (meters above sea level).

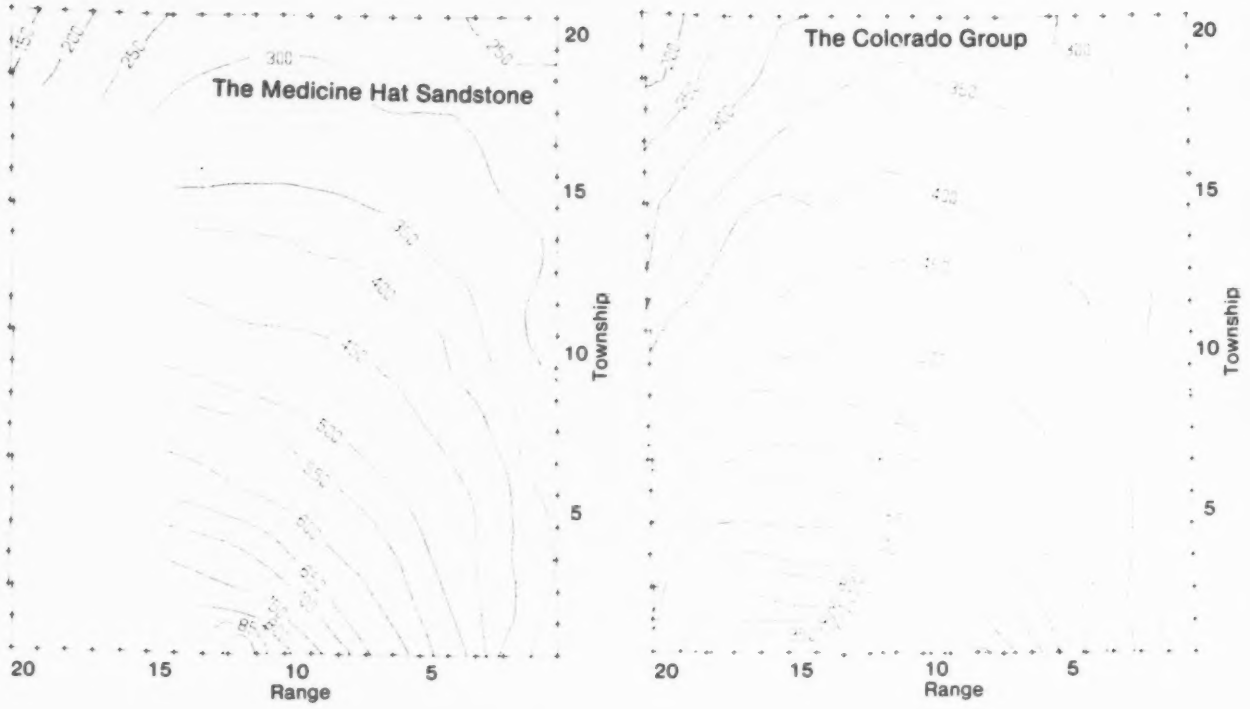

Figure 2.22 (continued)

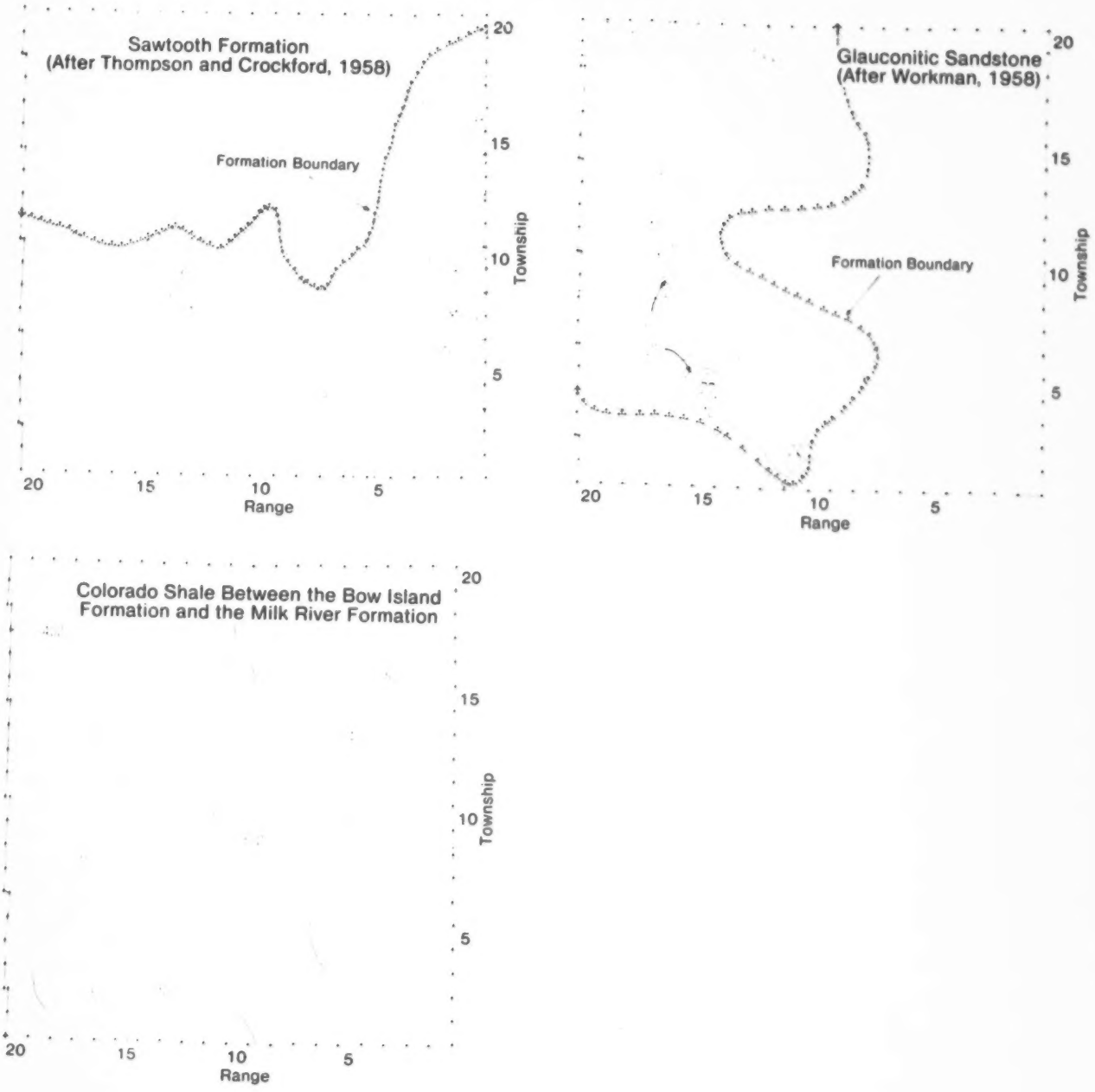

Figure 2.23 Map showing thickness of geologic units in southeastern Alberta (thickness in meters).

The Rierdon Formation consists of interbedded gray and green, calcareous to slightly calcareous shale, brown limestone and occasional gray-green argillaceous siltstone (Thompson and Crockford, 1958). The Swift Formation is a dark brown to gray shale which overlies a glauconitic brown shale. The shale grades upward into fine silty sand finely interbedded with dark bituminous shale (Thompson and Crockford, 1958). The Swift Formation is limited to the southeastern corner of the study area.

Jurassic sediments were, for the most part, laid down by shallow advancing seas (Thompson and Crockford, 1958). Uplift of the Sweetgrass Arch resulted in erosion of most of the Jurassic along the crest of the arch. Jurassic sediments thicken east and west of the flanks of this structure. Figure 2.22 shows structural contours on the top of the Jurassic.

The Cretaceous Mannville Group overlies the Jurassic over most of the study area except in a small zone along the northern boundary where it overlies Mississippian beds. The Mannville Group consists of the Cutbank Sandstone, the Sunburst Sandstone, the Ostracod Zone, and the Glauconitic Sandstone.

Cutbank Sandstone is a fine to medium grained quartz sand. The sand grains are subrounded and cemented by silt and secondary quartz (Blixt, 1941). The chert content and mean grain size increases towards the base of the unit. Conglomerates generally occur near the base (Glaister, 1958).

Sunburst Sandstone is depositionally continuous with the Cutbank Sandstone. It is medium grained, composed of rounded quartz grains that in places exhibit secondary overgrowths, and contains minor amounts of chert and argillaceous material. The clay matrix is highly variable and gives the unit an irregular distribution of porosity. In the northern part of the study area, the Sunburst and Cutbank Sandstone may be separated by a red to green shale up to 6 m thick (Glaister, 1958).

The Ostracod Zone overlies these basal sandstone units. It consists of a thin shale, siltstone or strongly cemented calcareous sandstone, capped by a thin argillaceous limestone. The Glauconitic Sandstone overlies the Ostracod Zone and consists of very fine to medium grained marine sandstone with varying amounts of glauconitic and argillaceous material. The average thickness ranges from 15 to 25 m, however, the sandstone is highly lenticular (Figure 2.23). The matrix is usually kaolinitic and constitutes 30 to 50 percent of the sandstone (Glaister, 1958).

Above the Glauconitic Sandstone, the Mannville Group consists of a non-marine sequence of gray silty shale, gray siltstone, argillaceous sandstone and thin coal beds (ASPG, 1966). At the east border of the study area this sequence is about 60 m thick. Structural contours on the top of the Mannville are illustrated in Figure 2.22.

The Cretaceous Colorado Group comprises all the strata between the top of the Mannville Group and the First White Specks. The Colorado Group is comprised predominantly of shale with minor interbedded sandstone units. Included in this group are the Basal Colorado Sand, Bow Island Formation, Fish Scale Sandstone, Second White Specks Formation, Medicine Hat Sandstone, and the First White Specks Formation. Structural contours on the top of the Colorado are shown in Figure 2.22.

The "Basal Colorado Sand" is a thin, 5 m thick, chert rich, fine to medium grained sandstone that pinches out to the north (Glaister, 1958). The Bow Island Formation is defined generally over the interval from the Basal Colorado Sand to the base of the Fish Scale Sandstone (Figure 2.17). It consists of a series of interbedded dark gray micromicaceous shale and gray, fine grained sandstone with scattered chert pebbles and a bentonitic matrix (ASPG, 1960). Feldspar, clay matrix and rock fragments generally increase in abundance towards the west. The matrix is commonly chloritic giving a greenish color to the sandstone (Glaister, 1958). A thick shale bed occurs between the base of the Fish Scale Sandstone and the top of the uppermost sandstone in the Bow Island.

The Fish Scale Sandstone is a thin, generally less than 5 m, "salt and pepper" sandstone that is characteristically poorly sorted, subangular to subrounded with calcareous cement and numerous fish scales. The fish scale sand marker horizon is taken as the base of the Fish Scale Sandstone (ASPG, 1960) and is easily recognizable on geophysical logs (Figure 2.19). Structural contours on the base of the Fish Scale Sandstone are presented in Figure 2.22.

Rocks between the Fish Scale Sandstone and the Second White Specks, approximately 60 to 90 m thick, are undivided and consist predominantly of siltstone and shale. The Second White Specks Shale contains minute specks of calcareous material (Meyboom, 1960). The shale at the bottom of this interval grades into sandy silt and eventually into very fine to fine sand over a very small vertical distance at the top of the Second White Specks. This thin sandstone yields gas at a small field within the study area.

Over most of the study area, the interval in the Upper Colorado Group between the top of the Second White Specks and the First White Specks consists of a 200 to 250 m thick relatively uniform dark gray marine shale with occasional bentonitic horizons. We have designated this unit as the potential host for a radioactive waste depository on the basis of its lithology, considerable thickness and depth beneath the ground surface. There are no sandstone units in the sequence except in southeastern Alberta where the Medicine Hat Sandstone is present near the very top of the shale.

The Medicine Hat Sandstone contains a sequence of silty very fine to fine sandstone up to 15 m thick which is encountered about 25 to 30 m below the top of the Colorado Group (Figure 2.22). The sandstone exhibits a gradual grain size decrease northward, westward and eastward from the zone of thickest sand deposits in the vicinity of the city of Medicine hat (Tp 12, Rg 5) (ASPG, 1966). The mean grain size of the sandstone generally increases toward its top where it is overlain by a calcite layer followed by a thin bentonite layer (Kendall and Simpson, 1974). McCord (1957) identifies the presence of a porosity barrier on the southwest margin of the sand.

Figure 2.23 shows an isopach map of the Upper Colorado Group shale above the Bow Island and below the Milk River Formations. This map shows that the shale has a thickness that varies between approximately 300 and 400 m and is continuous across the entire study area.

The Cretaceous Milk River Formation conformably overlies The Upper Colorado Group. The Milk River Formation, by convention, includes a lower transition zone that grades through a series of sandy shales or shaly sandstones into an overlying massive sandstone (ASPG, 1966). These massive sandstones are fine to medium grained and commonly contain thin bands of lignite and ironstone concretions. The top of the bed is marked by a zone of black chert pebbles at the base of the overlying Pakowki shale. Across the southern portion of the study area, the Milk River Formation is an important but not very productive artesian aquifer.

The Pakowki Formation conformably overlies the Milk River Formation. It consists of dark gray marine shale interbedded with thin silty sandstone and bentonite beds (ASPG, 1966). The Pakowki shale is easily recognizable on geophysical logs (Figure 2.19). In southwestern Saskatchewan, it is over 150 m thick; northeast of Medicine Hat, it is approximately 250 m thick. The upper contact is gradational with the overlying Belly River Formation.

The Belly River Formation, in the study area, is composed of a lower member, the Foremost, and an upper member, the Oldman. The Foremost Member is comprised of gray and dark gray shale, coal seams, and thin sandstone beds. The Oldman is typically comprised of light colored shale and sandy shale with some coal beds.

The Bearpaw Formation, which conformably overlies the Belly River Formation, is predominantly composed of dark gray marine shale with a few thin sandstone and bentonite beds. The Bearpaw is the stratigraphic equivalent of the upper part of the Pierre Shale of South Dakota. Bedrock and glacial drift units overlying the Pakowki Formation have not been subdivided on the fence sections (Figure 2.18) and in the stratigraphic column (Figure 2.17).

2.4.3 *Properties of Geologic Units*

2.4.3.1 *Hydrologic Properties* - Sufficient information is available to develop a reasonably accurate picture of the hydraulic conductivity distributions in the non-shale portions of the stratigraphic sequence. In this respect the data base for the western Canada sedimentary basin is far superior to that of the other basins examined. Hydraulic conductivity values are determined from approximately 590 drill-stem tests and 35 aquifer tests within the study area. Basic drill-stem data were obtained from the Energy Resources Conservation Board of Alberta and were interpreted using standard methods (Earlougher, 1977). Permeability values are calculated from a knowledge of flow rate, formation volume factor, viscosity, packer spacing and the change in shut-in pressure per log cycle. For comparative purposes, the permeability values are converted to hydraulic conductivity values assuming the pore fluid is water at 15°C.

In Figure 2.24, histograms are used to summarize the hydraulic conductivity data for the 7 main sandstone units and 1 limestone unit within the stratigraphic sequence. For each unit, the number of samples tested is shown in the figure. The number tested ranges from 18 for the Glauconitic Sandstone to 146 for the Bow Island Sandstone. Qualitatively, it appears that the mean hydraulic conductivity correlates with the mean grain size of the sandstone units. The fine to medium grained sandstones (Sawtooth, Sunburst, Glauconitic) have a relatively higher mean hydraulic conductivity than the very fine grained to fine sandstones (Second White Specks, Medicine Hat). Clay content and cementation contribute to the reduction of the mean hydraulic conductivity for several units, the most notable being the Bow Island, Medicine Hat, and Milk River Sandstones. The hydraulic

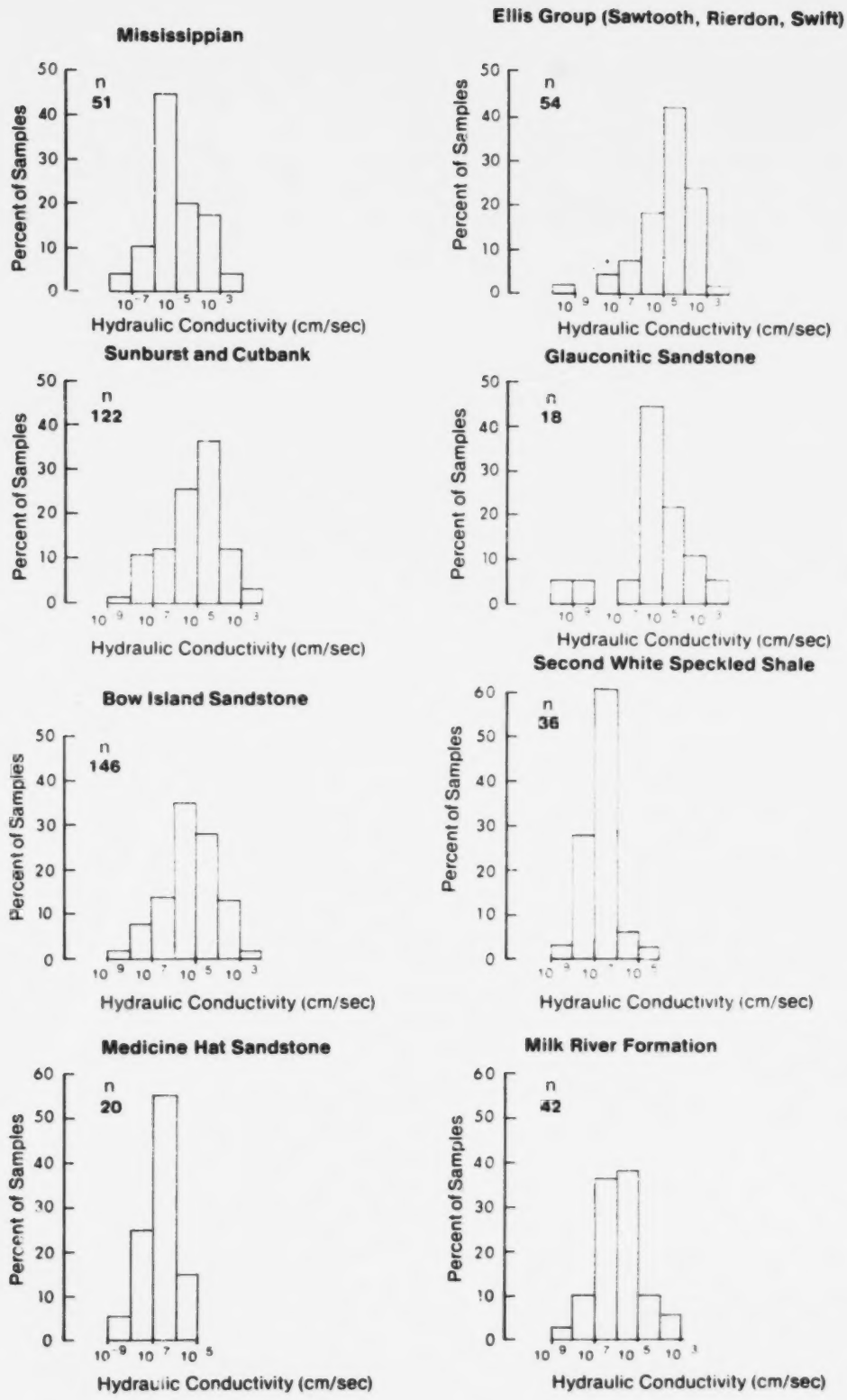

Figure 2.24 Histograms of hydraulic conductivity of geologic units in the western Canada sedimentary basin.

conductivity of the sandstone units is actually quite low relative to commonly reported values. In the entire Cretaceous sequence, only the southern portion of the Milk River Formation has what could be considered to be moderately high conductivity.

Porosity data are available for nearly all the units for which hydraulic conductivity histograms are presented. With the exception of the Mississippian units, values range from 15 to 20 percent. Mean porosity for the Mississippian dolomite and limestone is approximately 10 percent. It remains uncertain to what possible extent fracturing of the rock units has been responsible for the development of the effective porosities. The low porosity of the Mississippian carbonates coupled with relatively high hydraulic conductivity suggests that fracturing might be significant. However, additional work will be necessary to evaluate the extent of fracturing in different units. Porosity data are not available for the shales of the Upper Colorado Group. No drillstem test data, hence no hydraulic conductivity data, are available for deeper shales in the stratigraphic section. However, from values obtained for shales in the Illinois and Williston Basins and from values reported elsewhere (Davis, 1969; California Dept. Water Resour., 1971; Freeze and Cherry, 1979), it can be expected that the shales would have hydraulic conductivity values less than 10^{-6} cm/sec and probably less than 10^{-8} cm/sec. Schwartz (1975) used the results of drawdown response tests with piezometers at depths less than 100 m to estimate the hydraulic conductivity of shale units in the Oldman Member. The mean of six determinations was 2×10^{-7} cm/sec.

Hydraulic conductivity data are plotted in Figure 2.25 as a series of maps to illustrate the spatial variation in this parameter. The Mississippian is characterized by a relatively high hydraulic conductivity zone trending northwest-southeast (Figure 2.25). This trend coincides closely with the west flank of the Sweetgrass Arch. Because the arch was uplifted in Jurassic time, tectonic stresses may have caused fracturing of the Mississippian limestone and dolomite to produce the high hydraulic conductivities. The west- to east-trending high conductivity zone in the Sawtooth Formation corresponds to thicker deposits of the unit (Figure 2.23) within a saddle of the Sweetgrass Arch (Thompson and Crockford, 1958). In addition, the sediments here generally have a lower clay content. The Sunburst, Glauconitic, and Bow Island sandstones appear to possess a comparable high hydraulic conductivity zone that appears to correspond to zones of higher sand content (ASPG, 1966). The lenticular nature of the Glauconitic Sandstone (see Figure 2.23) is evident in the spatial variation of hydraulic conductivity. Areas with a relatively high hydraulic conductivity are apparently isolated.

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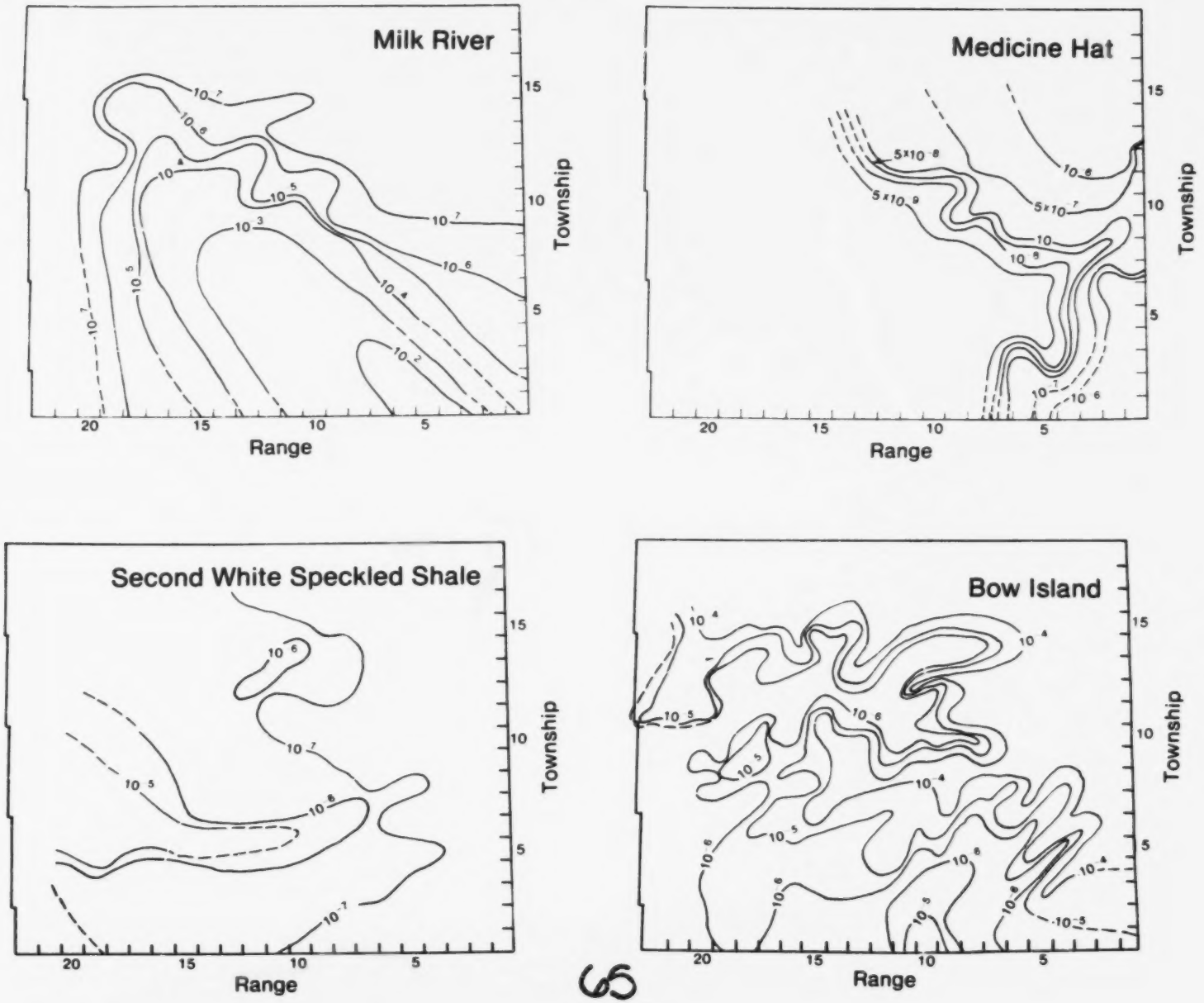


Figure 2.25 Maps showing spatial variation of hydraulic conductivity in geologic units in southeastern Alberta. Conductivity units are cm/sec.

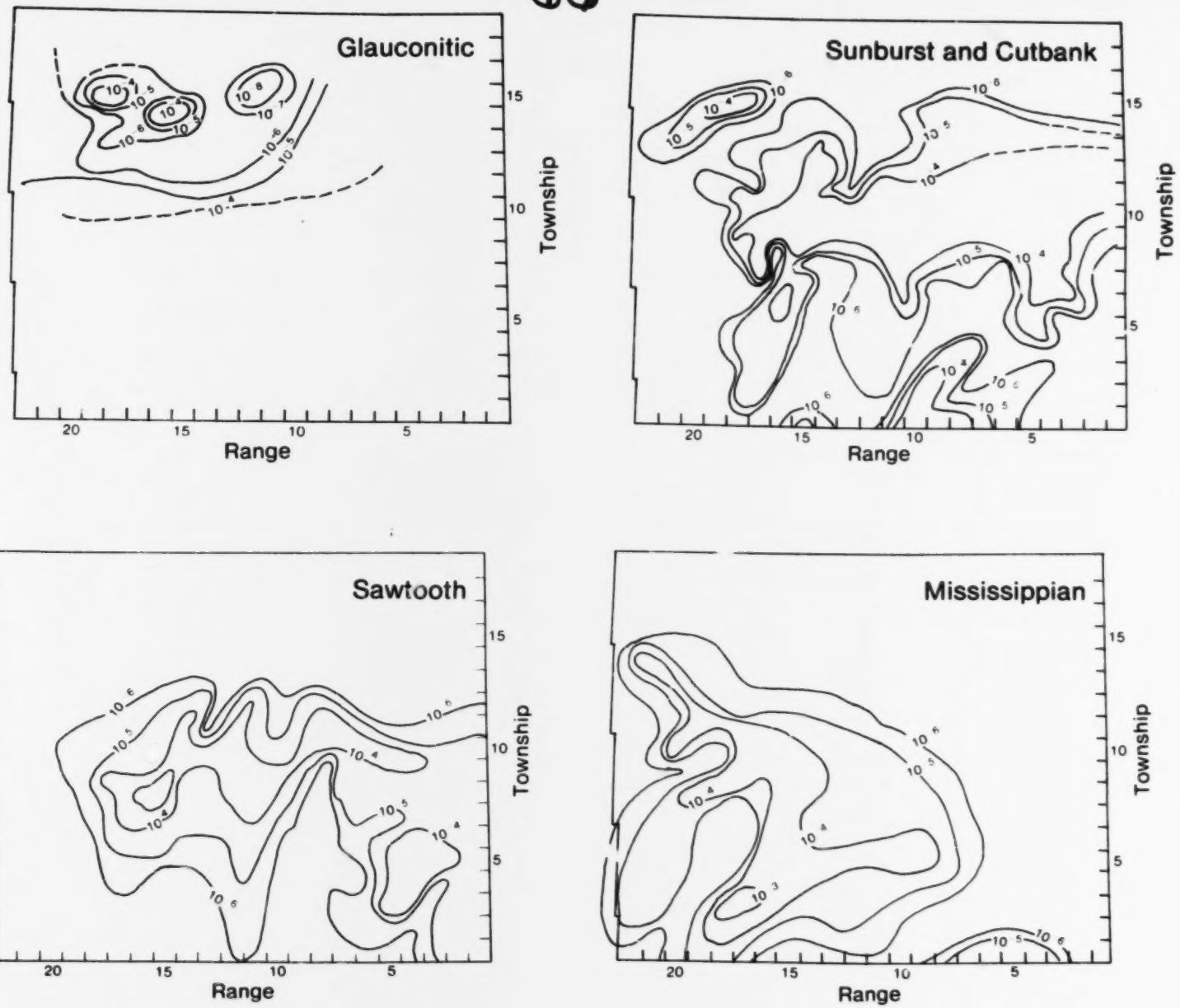


Figure 2.25 (continued)

The hydraulic conductivity of the Medicine Hat Sandstone generally decreases towards the southeast (Figure 2.25). This trend is produced by an increasing proportion of shale in the formation in that direction (McCord, 1957). Highest values of hydraulic conductivity occur in the area of maximum sand thickness.

The Milk River Formation displays a northwest-southeast trend in hydraulic conductivity. This pattern is a result of the increasing proportion of shale in the formation to the north and the variable thickness of sandstone beds (Meyboom, 1960).

2.4.3.2 *Geochemical Properties* - Clay mineral compositions of sandstones of the Lower Cretaceous are largely comprised of kaolinite with lesser quantities of smectite (Glaister, 1958; Carrigy and Mellon, 1964). In addition to these clay minerals, the Lower Cretaceous Bow Island Formation contains chlorite which imparts a greenish color.

Smectite and mixed-layer clays are important in the Upper Cretaceous Fish Scale, Medicine Hat, and Milk River Sandstones. The Fish Scale Sandstone also contains substantial amounts of illite with minor kaolinite. The Milk River and Medicine Hat both have minor amounts of kaolinite and illite (Black et al., 1980). Smectite and mixed layer clays have the greatest attraction for water and exhibit the highest degree of swelling of all the common clays. During drilling operations, this swelling can cause reduction of the permeability by plugging of pore spaces (Black et al., 1980).

Hoffman and Hower (1979) show that the dominant clay mineral in the Cretaceous shale is a mixed-layer illite-smectite which is randomly interstratified with a large portion of smectite layers. Bentonite beds within the Cretaceous contain a fully expandable smectite as the dominant clay mineral and have low potassium contents (Hoffman and Hower, 1979). Kaolinite and/or smectite are also the dominant clay minerals in the Tertiary sandstones (Carrigy and Mellon, 1964).

Data are not available for several important geochemical parameters that should be known for a complete characterization of the geochemical environment in the host rock and adjacent strata within the study region of the western Canada basin. Cation exchange capacities of upper Cretaceous shales in the basin have not been measured. A high smectite content in most of the shales and a high content of clay-size particles suggest that the units probably have high exchange capacities, perhaps similar to the Pierre Shale, and probably higher than the illitic shales of the

Illinois Basin. However, exchange capacity cannot be quantified from a mineralogic analysis. The pH and Eh of the system have not been measured. The presence of carbonate minerals in the system usually indicates that the pH is above neutral. The Eh of the system is unlikely to be oxidizing except very near the surface and perhaps slightly deeper in the aquifers near their surface recharge area. All other parts of the natural system should be in a reducing environment. The organic matter content of the shale units has not been measured; however, descriptions suggest that most of the shale units do not contain a high content of organic carbon. Although organic carbon is undoubtedly present throughout the shale units, most of the shale probably contains less than 1 percent organic matter. Petroleum accumulations occur in economically recoverable concentrations in several of the sandstone units. There are no trace element analyses that would identify the presence and quantity of naturally occurring radionuclides in the shales. Measurements of distribution coefficients are rare for argillaceous rocks, in general, and none have ever been determined for the various radionuclides in shales from the western Canada sedimentary basin. Ground-water chemistry is discussed in section 2.4.4.3.

2.4.3.3 *Thermal Properties* - To our knowledge, the only measurements that have been made of the thermal properties of sedimentary strata in the study area or its vicinity are those thermal conductivities shown in Table 2.7. There are no available measurements of expansion coefficient or heat capacity. Geothermal gradients have been measured in the region and determined to range from about 31 to 33°C/km (Magara, 1976). This gradient is similar to that in the Williston Basin and higher than in the Illinois Basin. The mean annual surface temperature of the area is about 5°C. Using this information, it can be expected that temperatures at repository depths between 300 and 1000 m might range from about 14.3° to 38°C.

2.4.3.4 *Mechanical Properties* - A survey of all available literature and discussion with experts who are working in the basin indicates that there are no data for mechanical properties of geologic units in the region studied or its vicinity. Geologic descriptions of the shale units suggest they are moist, porous, weak, poorly compacted, clay shales rich in smectite minerals. They probably have mechanical properties similar to the Upper Cretaceous Pierre Shale of South Dakota. Beyond obvious lithologic and mineralogic similarity to the Pierre, they, like the Pierre, have probably not been deeply buried or subjected to abnormally elevated temperatures since their deposition.

Table 2.7 Thermal conductivities of geologic units in the western Canada sedimentary basin (modified from Garland and Lennox, 1962).

Geological Unit	Lithology	Thermal Conductivity $Jm^{-1}sec^{-1}{}^{o}C^{-1}$	Number of Samples
Pakowki Fm.	shale	1.55	1
Colorado Gp. over 2nd White Speck.	dense hard shale	1.55	1
2nd White Speck. Shale	dense hard shale	1.00 - 2.42	6
Bow Island Fm.	silty shale	2.09 - 5.06	3
	dense shale	2.17	1
	soft carb. shale	0.92 - 2.51	3
Mannville Gp. above Glauc. ss.	sandstone	1.30 - 3.22	3
	silty shale	1.30 - 1.84	3
Glauconitic ss.	sandstone	1.30 - 4.93	3
	sandy shale	4.18 - 6.40	3
	dense shale	2.22 - 3.72	2
Mannville Gp. below Glauc. ss.	sandstone	1.67 - 3.05	3
	silty shale	3.60 - 6.31	2
	dense shale	2.30	1

2.4.4 *General Hydrologic Conditions and Setting*

2.4.4.1 *Hydraulic Head Distribution* - Detailed hydraulic head distributions have been determined mainly from extrapolated drill-stem pressure data. These data far exceed in number the data available for the Illinois Basin, and because we have been able to obtain original test records, they far exceed in quality the data available for the Williston Basin. In all instances, test results have been rejected if the initial and final maximum pressures differed by more than 5 percent. Pressure determinations are expressed as equivalent fresh water head in meters above sea level at 15.6°C (Schwartz et al., 1980). Maps of the potentiometric surfaces have been prepared from this data set and are illustrated in Figure 2.26. Because these surfaces might be influenced by gas and oil production (or ground water in the case of the Milk River aquifer), the location of major fields is indicated on the figure.

2.4.4.2 *Ground-Water Flow Pattern* - It is difficult to determine the extent to which gas, oil, and/or water production has influenced hydraulic head distributions in the various units. There is evidence of local depressions in the potentiometric surfaces for the Bow Island, Milk River and Mississippian units (Figure 2.26). Widespread and anomalously low values of hydraulic head in the Bow Island Formation, and to a lesser extent in the Milk River Formation, suggest significant changes from the virgin reservoir conditions. Depicted in Figure 2.26 are the interpreted flow conditions for eight major geologic units. Although there is a certain amount of scatter in actual direction, a consistent pattern of flow from south to north is present. This pattern appears to be preserved even in the Bow Island and Milk River Formations. As will become clear in later sections, such a flow pattern is supported by the existing geochemical data. In addition, these results are in agreement with those presented by Hitchon (1964, 1969a, 1969b) for much of the western Canada sedimentary basin. The continuity of the head fields confirm Hitchon's observations that very large ground-water flow systems exist in the basin.

Detailed examination of data from the Bow Island Formation, Sunburst Sandstone, and Mississippian illustrates how the patterns of flow are controlled by the variation of hydraulic conductivity (compare Figure 2.25 and 2.26). For example, in the case of the Bow Island Formation the tendency for ground water to flow in a northeasterly direction is related to the location of a conductivity high.

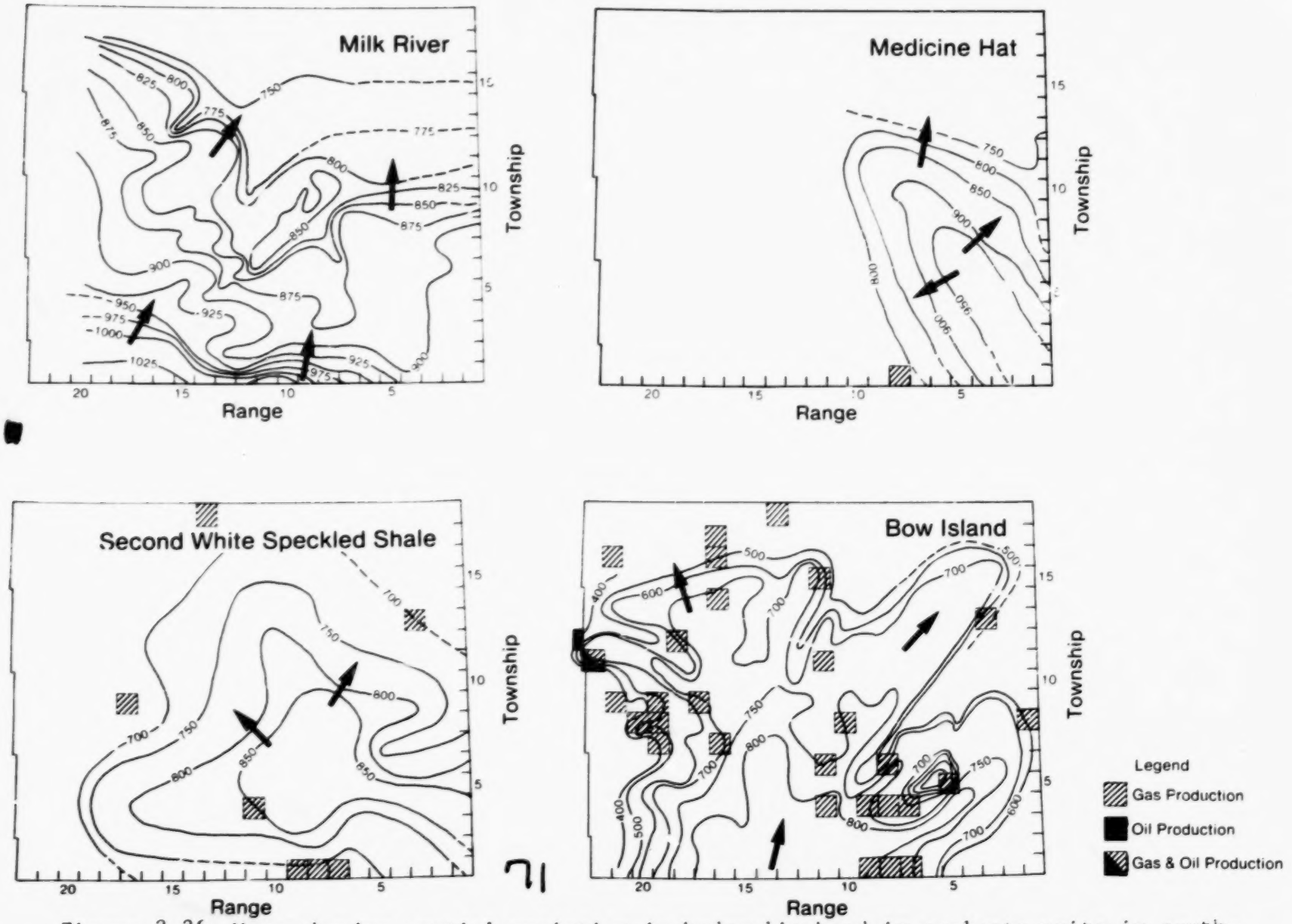
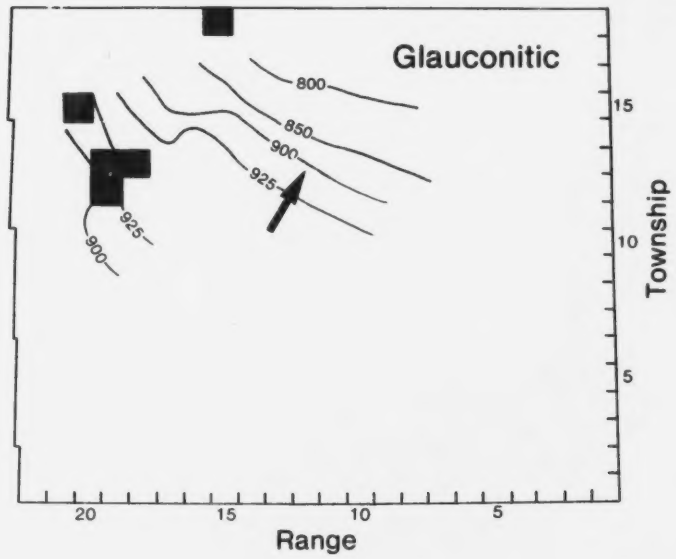
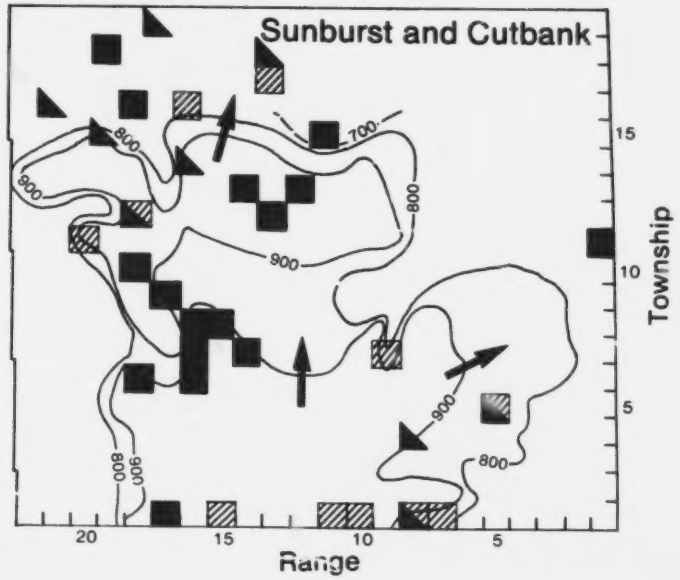
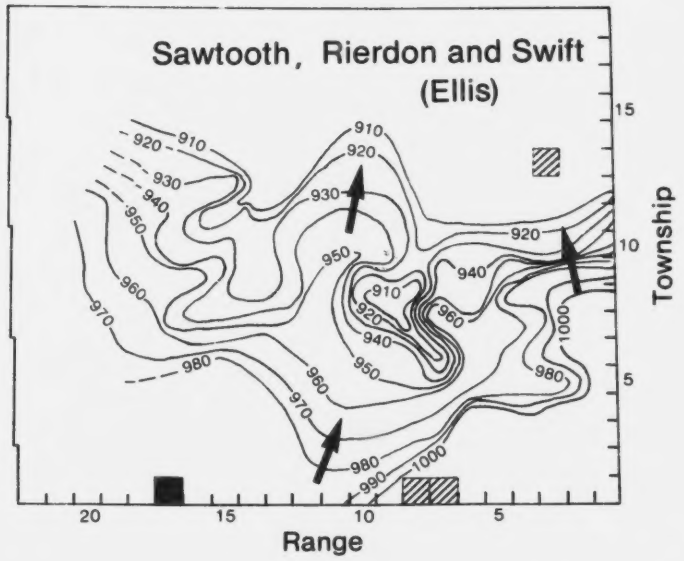
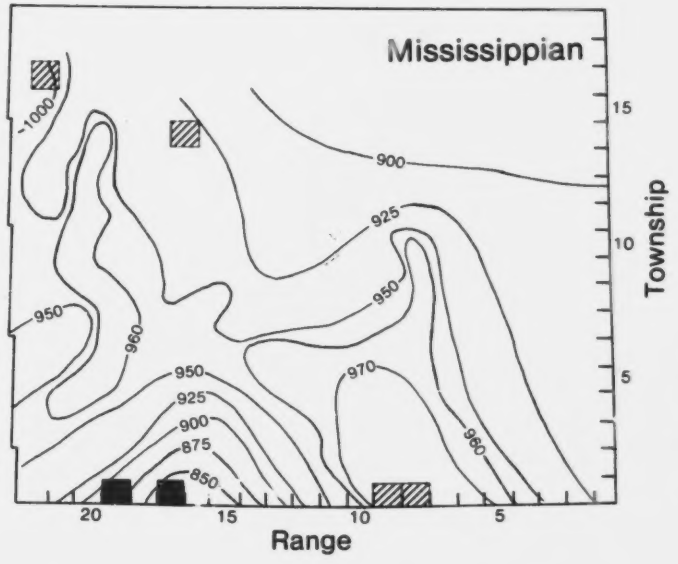


Figure 2.26 Maps showing spatial variation in hydraulic head in geologic units in southeastern Alberta.









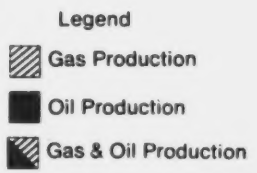


Figure 2.26 (continued)

Evaluation of the vertical flow components is difficult because head calculations from drill-stem test data probably have errors associated with them which are the same order of magnitude as the actual vertical differences in head. It is possible, however, to make certain generalizations. The Milk River is recharged along its outcrop area in the southern portion of the study area. North of the recharge area, flowing wells completed in the Milk River aquifer provide good evidence that water is moving upward toward the surface. It is probable that quantities of water are also leaving the aquifer from the bottom and moving downward. The Bow Island Formation appears to be a head potential low with flow directed upward toward it from below and downward from above. These low heads are in part the result of long term pumping of petroleum, which began in the Bow Island in the 1920's. The relatively high hydraulic conductivity values of the sandstone units in the sequence as compared to the shale units suggests that flow should be generally nearly horizontal in the sandstone units and vertical in the shale or siltstones (Neuman and Witherspoon, 1969).

2.4.4.3 *Ground-Water Chemistry* - The geochemistry of formation water in the study area has been studied extensively by Schwartz and Muehlenbachs (1978) and Schwartz et al. (1980). We will describe the distribution of Na^+, Cl^-, and SO_4^{2-} ions, which are the most dominant major ion species, and the stable isotope ratios of D/H (Deuterium/Hydrogen) and $^{18}O/^{16}O$. The isotopic data are discussed not because of their significance with respect to possible radionuclide transport, but because they have proven to be of enormous value in tracing the ground-water flow systems. The basic data for the ion chemistry are approximately 240 good quality unpublished analyses of water samples, which were obtained mainly from drill-stem tests but also from a few separators. These data are supplemented by approximately 1500 analyses of formation water which were collected over the last 20 years and kept on file with the Energy Resources Conservation Board of Alberta. An additional 93 good quality analyses are available for water from the Milk River aquifer.

The distributions of Na^+, Cl^-, and SO_4^{2-} ions are shown in Figures 2.27, 2.28, and 2.29 for the Milk River Formation, Bow Island Formation, Mannville Group, and Sawtooth Formation. We believe that the maps accurately reflect the major variations in Na^+, Cl^-, and SO_4^{2-} ion concentrations because:

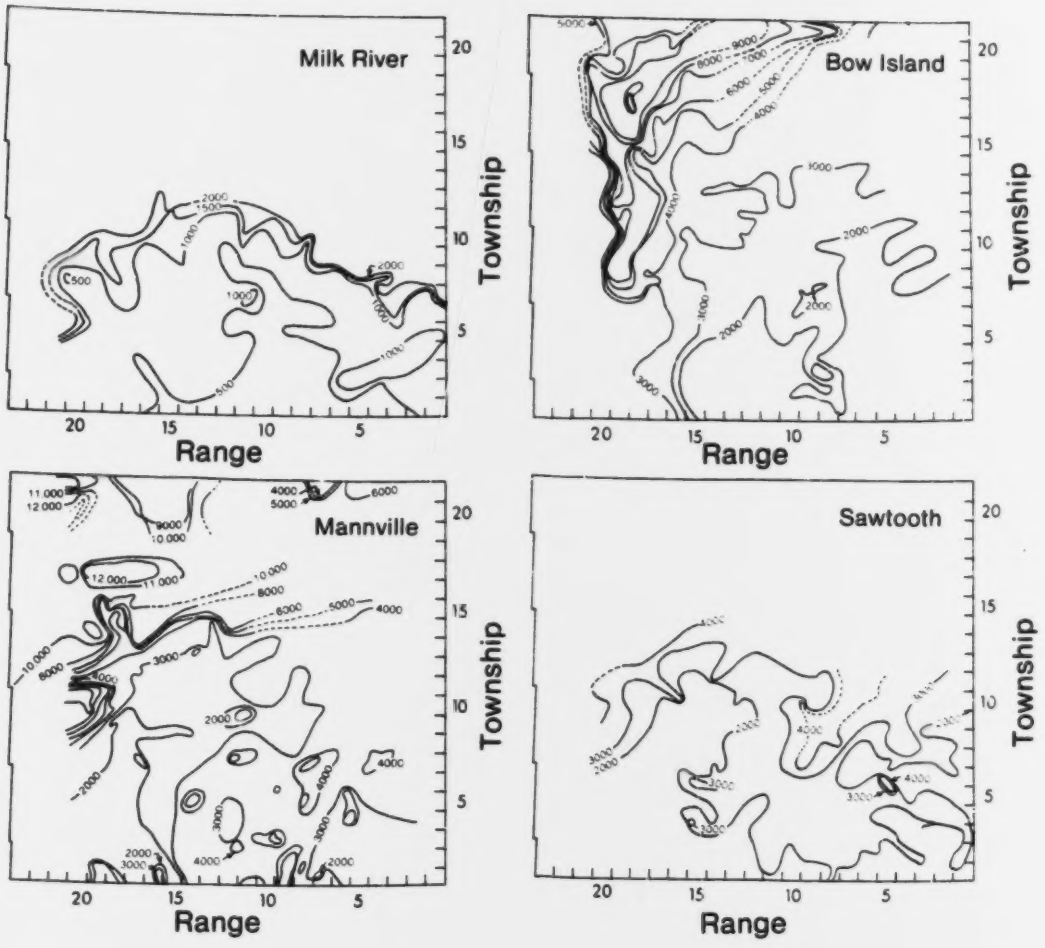


Figure 2.27 Maps showing Na^+ ion concentration (mg/l) in ground water in southeastern Alberta.

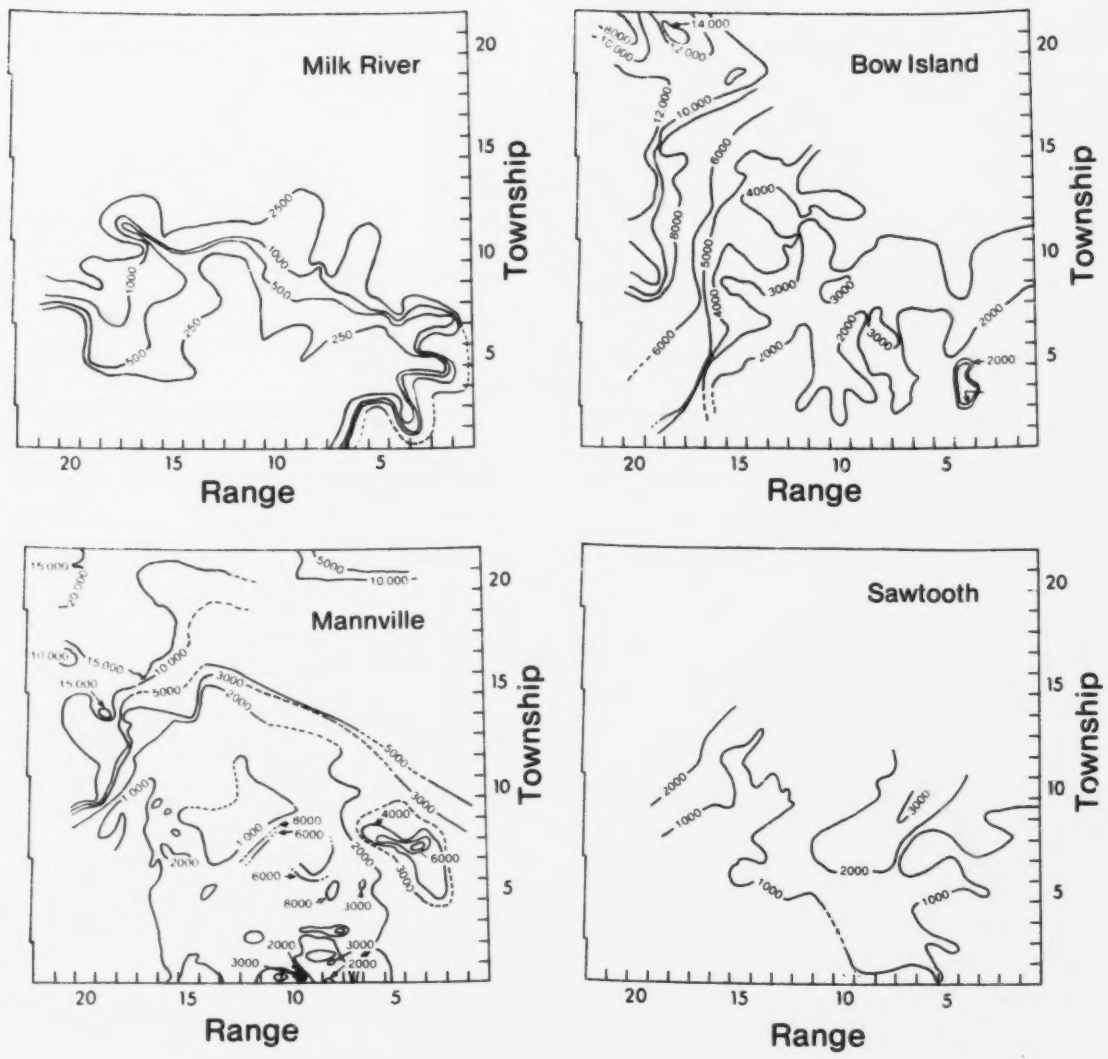


Figure 2.28 Maps showing Cl^- concentration (mg/l) in ground water in southeastern Alberta

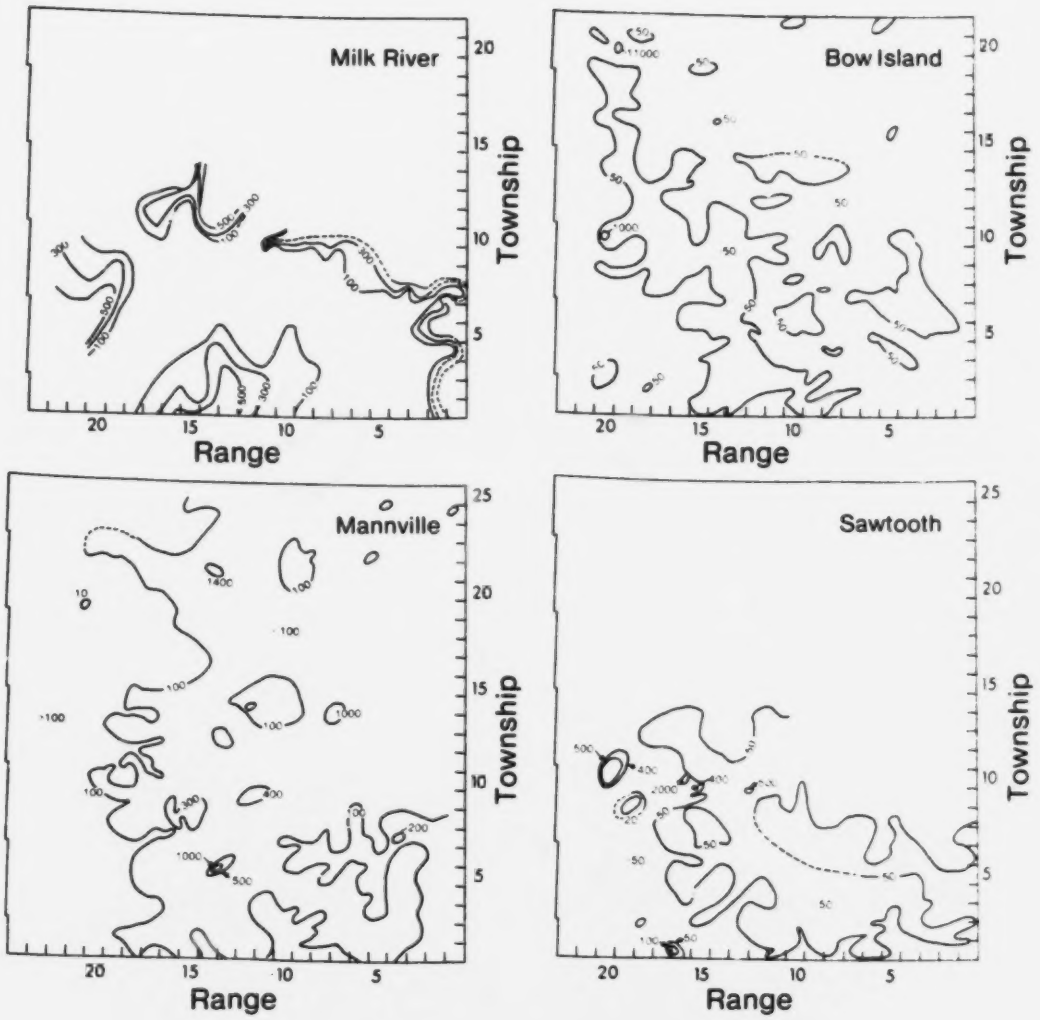


Figure 2.29 Maps showing SO_4^{2-} ion concentration (mg/l) in ground water in southeastern Alberta.

1) each of the maps is based on a relatively large number of data points;

2) the data are reasonably consistent in any given area of each map; and

3) the trend of increasing concentrations is completely compatible with the hydrodynamic data.

However, we had no control over the collection or analysis of these samples and, as a result, are not able to evaluate more specifically the possibility for errors in the results such as might be by sample contamination by drilling fluids.

In the case of Na^+ concentrations, all formations show a systematic increase from south to north across the study area (Figure 2.27). Values in the Milk River aquifer range from approximately 500 to 2000 mg/l. In the Bow Island Formation and the Mannville Group, Na^+ concentrations are higher, ranging from approximately 2000 to more than 8000 mg/l. Sodium ion concentrations in the Sawtooth Formation may be somewhat higher (Figure 2.27). Concentrations of Cl^- in the Bow Island reach a maximum of 14,000 mg/l; while, those from the Mannville reach a maximum of 20,000 mg/l (Figure 2.28). For the SO_4^{2-} ion, patterns are more complex. Typically, values for the Milk River aquifer are less than 100 mg/l except in areas along the edge of the aquifer (Figure 2.29). Concentrations in the Bow Island Formation are typically less than 50 mg/l except to the west. A similar pattern is evident within the Mannville Group, with values to the west greater than 100 mg/l (in a range from approximately 100 to 800 mg/l) and those to the east less than 50 mg/l (with the exceptions indicated). In the Sawtooth Formation sulfate concentrations are variable, making it very difficult to subdivide regions in which the concentration is greater than 50 mg/l.

The ^{18}O and D values are determined for 118 formation water samples from various units in the stratigraphic section. Most of the 39 samples from the Milk River Formation were collected from water wells (Schwartz et al., 1980). The remainder are drill-stem test samples gathered in a detailed program of studies sponsored by the Alberta Research Council and The Energy Resources Conservation Board of Alberta.

For those geological units for which sufficient samples are available (i.e. Milk River Fm., Bow Island Fm., Sunburst Sandstone, and Sawtooth Fm.), it is possible to describe systematic variations in D and ^{18}O (Figures 2.30 and 2.31). The most marked variations are observed for the Milk River aquifer where δD values range from -150 parts per thousand (‰) to greater than -90‰ and $\delta^{18}O$ values range from less than

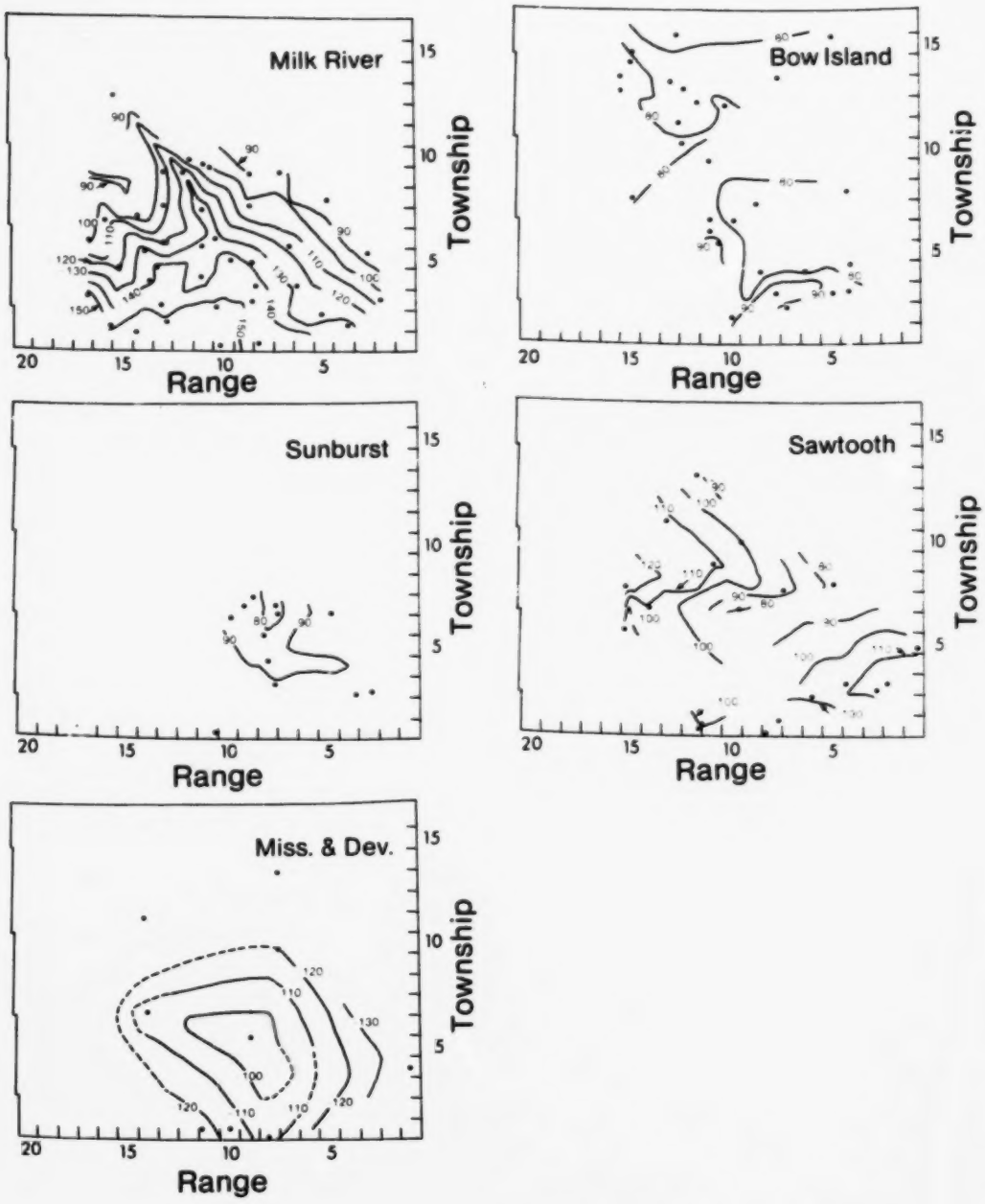


Figure 2.30 Maps showing variations in δD (‰) in ground water in southeastern Alberta.

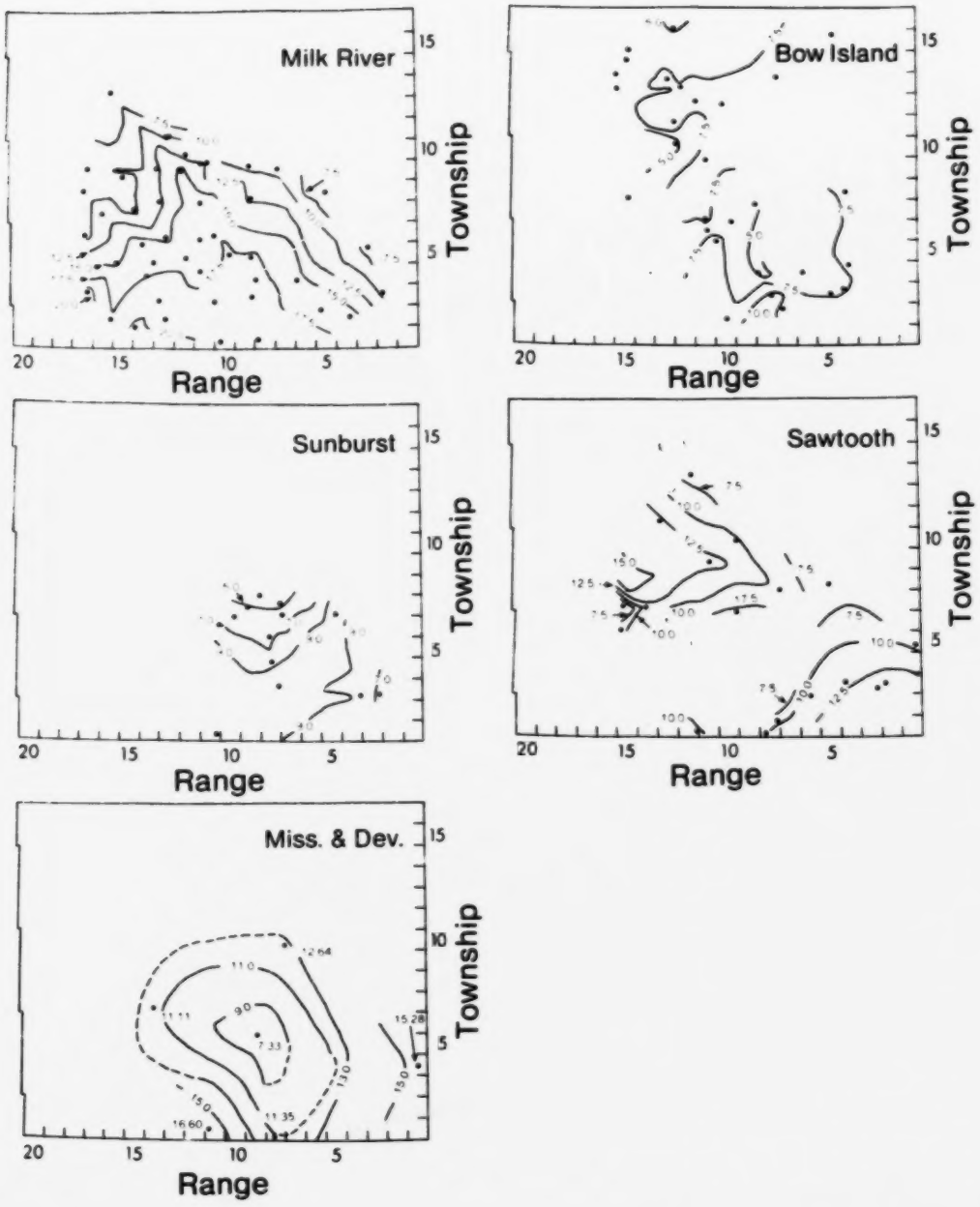


Figure 2.31 Maps showing variations in $\delta^{18}O$ (‰) in ground water in southeastern Alberta.

-20‰ to greater than -7.5‰. Formation water from the Bow Island Formation generally falls within a much narrower range. Deuterium contents have a maximum variation of approximately 25‰ and ^{18}O contents have a maximum variation of about 5‰ The range in variation for the Sunburst Sandstone is almost identical to that for the Bow Island (Figures 2.30 and 2.31). In the Sawtooth Formation, δD values vary from approximately -125‰ to -77‰ with many of the values less than -100‰. Oxygen-18 values range from about -16‰ to -5.5‰. Determinations for the Mississippian and Devonian units represent some of the lowest D and ^{18}O values for waters from units deeper in the section than the Milk River Formation.

The wide range of isotopic values for water from the Milk River Formation can be attributed to large scale mixing processes (Schwartz and Muehlenbachs, 1979). Meteoric water with a δD content of approximately -157‰ and a $\delta^{18}O$ content of approximately -20‰ displaces pre-existing formation water. Such a system has probably been operating for less than 15,000 years. Thus, flushing is incomplete and a zone of mixing remains between waters with very different isotopic concentrations.

No other formation contains isotopically unaltered meteoric water. However, the fact that these waters are mostly brackish and have δD contents of the range from -120 to -70‰ suggests that they are the result of long-term mixing of meteoric and connate waters. Hitchon and Friedman (1969) argued that such mixing could explain the isotopic character of shallow formation water in the western Canada sedimentary basin.

There appears to be an apparent correlation between the extent of mixing and the hydraulic conductivity of individual units. For example, the hydraulic conductivity of Mississippian units and the Sawtooth Formation are high relative to the Bow Island Formation. Indications from the D data are that these deeper and more conductive units contain a relatively higher proportion of meteoric water. This evidence suggests that flushing of formation water from the basin depends upon the broad scale features of hydraulic conductivity. The higher conductivity elements of the geologic system represent pathways along which meteoric water moves into the basin.

Examination of Na^+, Cl^-, and SO_4^{2-} ion concentrations in relation to the deuterium data shows that the concentration of these species is determined by the chemical evolution of water moving along the flow system. For example in the Bow Island Formation, the concentrations of Na^+ and Cl^- increase markedly in the direction of flow, whereas D contents remain within a narrow range. Similar relationships are evident in the Mannville units. Only in the Milk

River Formation is there an apparent relationship between Na^+ and Cl^- ion concentration and δD. However, it can be shown that the salinity of the water increases independently of deuterium concentration once values are greater than -100‰.

2.5 Summary Statement Regarding Areas Considered for the Reference Repository System in Shale

Of the three areas considered, the western Canada sedimentary basin has the most complete data base for defining the configuration of geologic units, characterizing the hydrologic properties of geologic units, and defining the ground-water flow regime. In addition, the thick shales and natural downward flow through the shales seem better suited as a repository system than either the Williston Basin, with its upward flow across the host unit, its incomplete data base for the configuration of geologic units, and its sensitivity to ground-water pumping, or the Illinois Basin with its incomplete hydraulic head and properties data base and poorly quantified flow system. Consequently, the western Canada sedimentary basin has been selected as the model for the reference repository system in shale (RRS-SH). Aspects of the characterization studies for the Illinois and Williston Basins contribute to the quantification of shale systems, in general, and will be used where needed to supplement the data base for the reference repository.

3. PRINCIPAL ASPECTS OF THE REFERENCE REPOSITORY SYSTEM

In this section we present a detailed quantitative description of the reference repository system for shale. The data which are tabulated here will form the basis for the flow and transport modeling to be presented in Section 4. It will become evident, however, that in spite of the relatively abundant information which is available for this portion of the western Canada sedimentary basin, relatively large gaps still remain in the data set. The areas of uncertainty include estimates of anisotropy, the state of fracture development, and transport parameters for the system. Such information is not commonly available from routine geological studies or from programs of petroleum exploration. Unfortunately, methods which can produce the necessary geological data from which to extract certain of the parameter values are not well developed.

3.1 The Ground-Water Basin and Boundaries of the Reference Repository System

One of the first important steps in modeling a natural system is the development of a row and column discretization of model parameters along a representative cross section of that system. Of interest here is the middle section of the fence diagram shown in Figure 2.18. This north-south section through the central part of the study area is parallel to the principal direction of ground-water flow in virtually all of the more permeable units (Figure 2.26). Thus, it is possible to model flow along this section using a two-dimensional model.

Three basic steps can be identified in the process of discretizing the natural hydrogeological system from a set of input data. Step 1 involves the definition of boundary conditions, a flow domain, and geological units in the section. Step 2 involves superimposing a grid on the reference section. Step 3 involves the assignment of parameter values (e.g., hydraulic conductivity) to each of the cells defined in the model. (See Figure 3.1.)

For the reference repository system in shale based on the western Canada sedimentary basin, we have specified constant-head boundaries along the top, bottom, and both sides of the flow domain. Such boundary conditions permit water and, in certain instances, contaminants to move across all four boundaries. This specification emphasizes that the domain is a part of a much larger flow system, and gives us flexibility in choosing the dimensions of the flow domain to be modeled. The real system extends, in fact, from Montana to northern Alberta. Here, we are model-

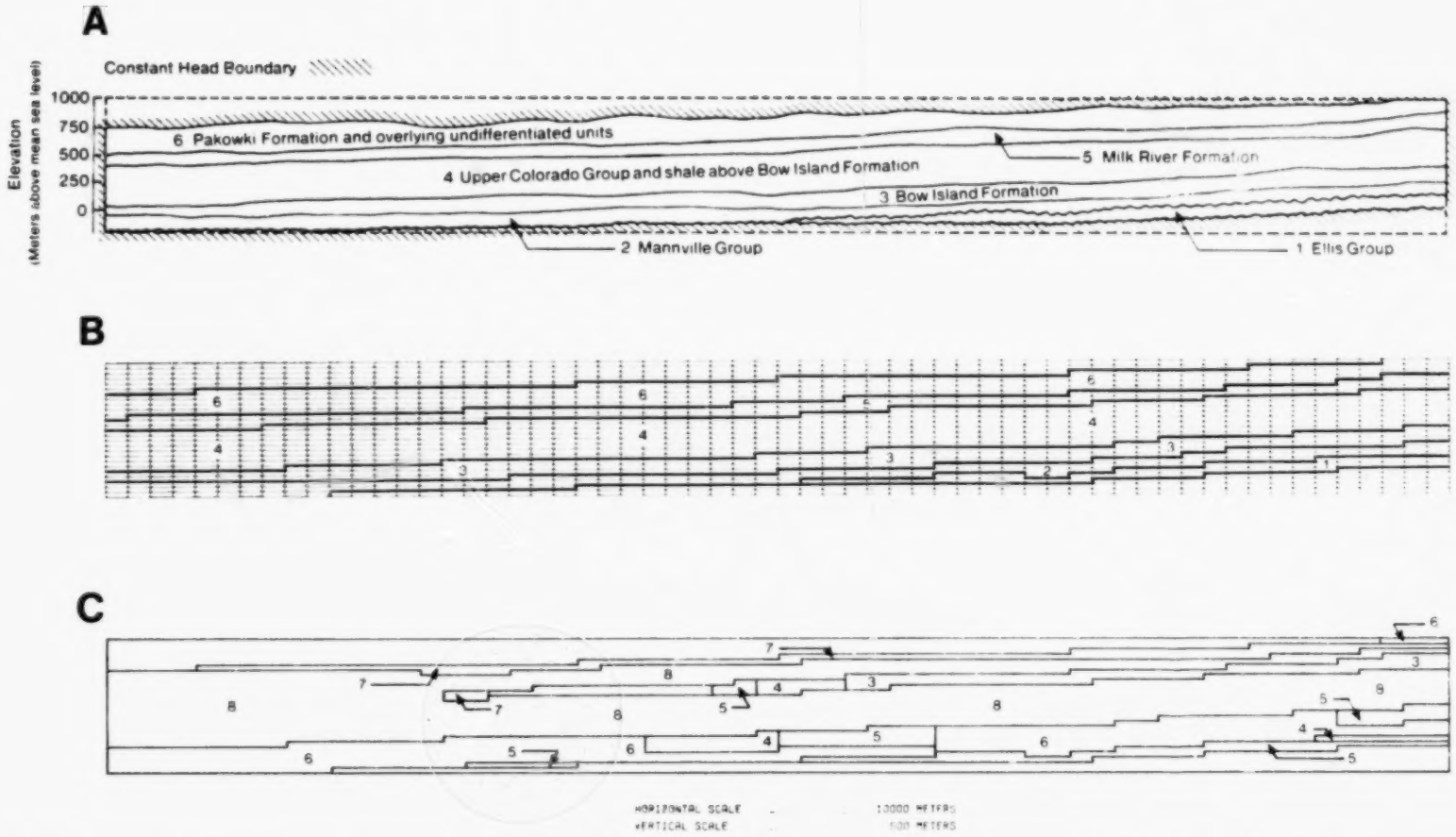


Figure 3.1 Three cross sections showing the sequential steps in (A) definition of boundary conditions, flow domain and geological units, (B) placement of the grid, and (C) assignment of values to properties of units for modeling ground-water flow and contaminant transport in the reference repository system.

ing a smaller part of that system, a section whose size is determined by the availability of the best quality data. However, this section (Figure 3.1a), termed the reference section, is sufficiently large to ensure that far-field effects on the spread of contaminants from the hypothetical depository are included in the simulations.

Values of hydraulic head assigned to the four boundaries are listed in the Appendix. Estimates for the bottom boundary are based on actual values calculated from drill-stem tests for the Mississippian and for the Ellis Group (Figure 2.26). The consistently high hydraulic heads in these units, as compared to the Bow Island Formation, suggest that the values are probably representative of virgin reservoir conditions. Values along the top boundary are determined by considering the water table to be a subdued replica of the ground surface (Tóth, 1962, 1963). Along the two sides, hydraulic head values are interpolated from the top and bottom boundaries.

Our concept of the reference repository system assumes that the natural conditions of flow do not change with time. The mathematical model for ground-water flow does not treat transients in flow created, for example, during construction of the repository, emplacement of the waste, or by pre-existing pertubations. Such transients would presumably be evaluated as part of the scenario evaluation to be made of the reference system. The fact that the hydraulic head distributions described previously for several of the units (Figure 2.26) have been affected by water, gas, and/or oil production means that existing hydraulic head data cannot be used in field verification of the flow models. Thus, we have no direct means of verifying the choices of hydraulic head or model parameters. This condition will likely be true for all reference systems and for all actual systems being evaluated as possible candidates for a waste isolation facility.

3.2 Configuration of Geologic Media

The stratigraphy along the reference section has been idealized to include only major units. Six units are defined that correspond generally but not exactly to stratigraphic units. These are not hydrostratigraphic units because values of hydraulic conductivity can vary in each. The stratigraphic equivalents of these major units are summarized in Table 3.1.

Step 2 in discretizing the hydrogeological system involves superimposing a grid on the reference section. The grid for the reference section is shown in Figure 3.1b. The

Table 3.1 Definition of stratigraphic equivalents of geologic units in the reference repository system.

Unit 6: Pakowki Formation and overlying undifferentiated units

Unit 5: Milk River Formation

Unit 4: Upper Colorado Group and shale in the upper Bow Island Formation

Unit 3: Bow Island Formation sand

Unit 2: Mannville Group

Unit 1: Ellis Group

section is subdivided by 27 rows and 61 columns, with each rectangular cell in the resulting set having a length of 2413 m and a height of 45.7 m. The numbering convention used here places Row 1 and Column 1 in the lower left hand corner of the grid.

The third and final step requires the various parameters, such as hydraulic conductivity or dispersivity, to be assigned to each of the cells. Because the horizontal component of hydraulic conductivity is one of the most important parameters controlling transport, we usually display its spatial variability together with hydraulic head data. Figure 3.1c illustrates the spatial variation in hydraulic conductivity used in initial modeling runs for the reference repository system.

3.3 Properties of the Geologic Media

In this section, values and ranges of values are assigned to properties of geologic units in the reference repository system. The specific values and ranges assigned were selected to represent to the greatest degree possible the natural geologic system as it exists in the western Canada sedimentary basin. It should be emphasized that at present no natural geologic system exists for which a "complete" data base can be compiled and used for the definition of a reference repository. Most properties of geologic and hydrogeologic systems must be measured with highly specialized tools and techniques designed specifically for the measurement being made. To adequately characterize an entire system, such tools and techniques must be applied in a standardized and repetitive fashion. There has been no incentive either in industry or in academia for such broad data acquisition, nor is there agreement on the tools or techniques best suited to the task. Thus, for the present, the reference repository system must be based on a natural system for which the most important aspects of the data base are most complete. Those aspects are the configuration of the geologic media, hydrologic properties of units, and head distribution. With this information the ground-water system can be evaluated. The ground-water system is the most important factor in system evaluation because it is the most likely means of transporting radionuclides to the biosphere. It should be noted that a "complete" data base probably won't exist until a natural system is characterized using state-of-the-art techniques for the specific purpose of assessing its suitability as a waste isolation system.

3.3.1 *Hydrologic Properties*

Values of horizontal hydraulic conductivity assigned to units 1, 2, 3, and 5 are based on field measurements (Figure 2.25). For units 4 and 6, no field measurements of hydraulic conductivity are available. The estimates for shale-dominated portions of the reference section are based on the possible range of values discussed in Section 2.4.3 and on the data available for the Pierre Shale (Section 2.3.3). Ranges of values for hydraulic conductivity are shown in Table 3.2.

Porosity values are assigned to units 1, 2, 3, and 5 on the basis of field determinations (see Section 2.4.3). As with hydraulic conductivities, no porosity data are available from the study area for the shale units, and values are assigned principally from data for the lithologically and mineralogically similar Pierre Shale (see Section 2.3.3). Ranges of values for porosities of units in the reference repository are shown in Table 3.2. Unfortunately, the existing data are insufficient to determine whether significant fracture porosity has developed in any of the units. Quantitative information on fracture development requires a much more sophisticated field testing program than has been carried out to date in the study area. In most site-specific investigations, uncertainty about the state of fracture development will be a major source of uncertainty in the predictive analysis of the confining capability of the geological system.

Following our previous practice, we assume that dispersion in media with anisotropic hydraulic conductivity can be characterized by a longitudinal and transverse dispersivity only (Schwartz and Donath, 1980). This simplification is justifiable because there is not a suitable model for anisotropic dispersion and because existing concepts of dispersion are themselves only rather crude approximations to what is a very complex phenomenon. No quantitative data are available to provide guidance in choosing a longitudinal dispersivity for the various units. As was the case for the reference repository system for bedded salt (Schwartz and Donath, 1980), a relatively small dispersion length (3 m) has been selected (Table 3.2). We believe that this magnitude is appropriate for contaminant plumes up to 1000 m in length. Transverse dispersion is assumed to be a fraction of the longitudinal value. In several studies (e.g., Bredehoeft and Pinder, 1973), the transverse value of dispersivity is commonly assumed to be 30 percent of the longitudinal value. However, recent theoretical (Smith and Schwartz, 1980) and applied studies (Sykes, 1980) would suggest that values of the order of 5 percent would be more appropriate for layered or other heterogenous media. Thus, in the reference repository transverse dispersivities of 0.12 m, or 4 percent of the longitudinal value, are used.

Table 3.2 Hydrologic properties of geologic units in the reference repository system.

		Hydraulic Conductivity (cm/sec)	Porosity (%)	Dispersion Length (m)
Unit 6.	Vert.	1.0×10^{-6} to 1.0×10^{-10}	15–30	3.0
	Horiz.	1.0×10^{-6} to 1.0×10^{-9}		
Unit 5.	Vert.	1.0×10^{-2} to 1.0×10^{-9}	15–20	3.0
	Horiz.	1.0×10^{-2} to 1.0×10^{-8}		
Unit 4.	Vert.	1.0×10^{-6} to 1.0×10^{-10}	15–30	3.0
	Horiz.	1.0×10^{-6} to 1.0×10^{-9}		
Unit 3.	Vert.	1.0×10^{-3} to 1.0×10^{-7}	15–20	3.0
	Horiz.	1.0×10^{-3} to 1.0×10^{-6}		
Unit 2.	Vert.	1.0×10^{-3} to 1.0×10^{-7}	15–20	3.0
	Horiz.	1.0×10^{-3} to 1.0×10^{-6}		
Unit 1.	Vert.	1.0×10^{-4} to 1.0×10^{-6}	15–20	3.0
	Horiz.	1.0×10^{-4} to 1.0×10^{-5}		

3.3.2 *Geochemical Properties*

The geochemical environment of a natural geologic system of the scale of the reference repository is very complex. Major geochemical factors important in determining the mobility of radionuclides in the reference system are poorly quantified in the existing data base. A number of generalizations can be made about the geochemical environment of the system, but there is, at present, insufficient basis for quantification of values or even a realistic narrowing of ranges of values for some important geochemical properties of the system such as the distribution coefficient (Kd), cation exchange capacity (CEC), or Eh.

Values for Kd are not available for radionuclides in shales of the western Canada sedimentary basin or for shales of the Williston or Illinois Basins. The distribution coefficient in the natural setting depends principally on the following factors:

1. mineral constituents in the rock
2. ground-water chemistry
   a. major and minor components
   b. Eh
   c. pH
3. radionuclide speciation and concentration
4. internal surface area
5. temperature

Each of these factors might vary spatially or temporally in the reference system. Mineral compositions are probably rather uniform within each geologic unit throughout the repository system, but differences in composition between units are substantial. Certainly, the quantity of clay minerals present varies greatly between shales and sandstones, and might do so between beds within units. The shales of the host unit are principally composed of smectite and mixed-layer illite-smectite. These minerals commonly exhibit high capacities for ion exchange. Thus, the shale units undoubtedly have the greatest potential for radionuclide sorption of all units in the system. Sandstones in the sequence contain substantially less clay, which also tends to be more illitic or kaolinitic than in the shales, and the sandstones therefore have lower potential for sorption. Pure smectite generally exhibits a CEC of about 100 milliequivalents per 100 grams (Tamura, 1972), and this value can be considered an upper limit to the possible range of CEC values exhibited by the host shales. The upper limit for the CEC of sandstones might be half that of the shales.

In the real system on which the reference system is based, there are large vertical and lateral variations in ground-water chemistry that might have substantial influence on radionuclide mobility. The ground-water chemistry has been discussed in detail in section 2.4.4.4. In general, the concentration of total dissolved species in the ground water increases with increasing depth and with increasing distance northward from the southern recharge area. This pattern of chemical variation in water chemistry suggests that deeper and more northerly portions of the system will exhibit decreased sorption of radionuclides caused by increased competition by stable ions for available exchange sites. Over the life of the depository the chemistry of the ground-water system should be expected to continue to evolve as it has in the recent geologic past. Connate waters will be further displaced as more and more meteoric water is recharged into the system. The extent and rate of this evolution cannot at present be predicted with confidence. Nevertheless, the distributions of CEC values within units of the reference repository system that are selected for use in scenario evaluation should take into consideration the natural variation, both spatially and temporally, that is implied by the preceding comments.

The pH and Eh of the system probably also vary regionally, but values for these parameters in the system are not specifically known. System pH probably falls within a range of 5 to 9 and might typically be neutral or slightly above. Most of the system is probably in a reducing environment (negative Eh). Penetration of oxidizing waters downward from the surface, especially in the southern region, is possible, but probably is restricted to shallow depths.

Methods used for most Kd determinations in the laboratory are such that generalizations cannot be made about values for Kd's in a complex natural system. Most column or batch measurements of Kd are conducted under oxidizing conditions, making the results of questionable value in predicting the behavior of certain radionuclides in the naturally reducing system. Often the permeabilities, flow rates, and sample surface areas used in column studies are several orders of magnitude higher than those that exist in the natural undisturbed system. In addition, temperature is usually about 25°C in column studies, but can range between 10° and 300°C or more in the natural system with nuclear waste in place.

Shales commonly contain organic matter in some form. In shales with a low temperature history, such as those of the reference system, the organic matter is usually present in the form of kerogen, a residue of finely divided organic material comprised mostly of macerated plant remains,

algae, spores, pollen, resins, waxes, and the like. For host shales of the reference repository, the total organic matter content, as inferred from the natural system, should probably be assumed to be 1 percent or less. Some of this material might be leachable in ground-water, and might thus affect radionuclide mobility by allowing complexing between organic molecules and ions. This effect cannot be quantified with available information. Thermal alteration of organic matter in the near-field of the depository could also occur, because temperatures in that region are likely to exceed those to which the shale has been exposed in the past. Such alteration could produce volatile gases, changes in porosity and permeability, and changes in fluid chemistry. These effects cannot be quantified with available information.

One final geochemical factor that might have significant influence on the migration of radionuclides in the repository system is that of osmosis. Osmotic pressures caused by chemical gradients across shale beds have been measured in laboratory studies and inferred in many field situations. In some instances, osmotic pressures might be sufficient to contain fluids in host rocks even where the permeability and hydraulic gradient data suggest movement would occur. This effect cannot be quantified for the reference system.

3.3.3 *Thermal Properties*

The most important single factor determining the manner in which a particular shale unit will respond to a given thermal load is the geologic thermal history to which it has been subjected. The thermal history is a product of the depth and duration of burial beneath overlying strata, and of the geothermal gradient. The maximum temperature to which a deposit has been subjected is rarely known accurately. However, in areas of relatively stable geothermal heat flow, the effects of thermal history can be approximated by analysis of the depth of burial and by assuming that the maximum temperature is directly related to the maximum depth of burial.

The host unit shales of the reference system have probably never been buried to depths greater than 1000 to 1500 m. Given the geothermal gradient in the system (31 to 33°C/km) and the average annual surface temperature (5°), it can be estimated that the shales have been exposed to temperatures no higher than about 38° to 55°C. This relatively low temperature history suggests that shales in this system might be more susceptible to alterations caused by the

thermal load of a depository than would shales with higher temperature exposure. Higher temperature histories could exist for natural shale systems of reasonable depths in regions where there are higher geothermal gradients or where deep burial was followed by subsequent erosion of overlying units. Targeting of actual sites for the possible location of a geologic depository in shale should take this into consideration.

Thermal conductivities of geologic materials in the natural setting are poorly known. Fortunately, results are available from a few laboratory determinations of the thermal conductivity of small samples of rocks from the western Canada sedimentary basin (Table 2.7) and can serve as a basis for assigning conductivities to geologic units in the reference repository. These data are consistent with measurements made on rocks from other areas. Shale units in the sequence have thermal conductivities that range from 0.92 to 6.31 J/m sec^{o}C. In general, the thermal conductivity of the shales increases with increasing density and sand content.

Dames and Moore (1978) examined data available on thermal conductivities of shale and suggested that a typical shale would have a range of thermal conductivity measured parallel to bedding of from 1.94 to 1.69 J/m sec^{o}C through a temperature range of 0^{o} to 400^{o}C, with conductivity decreasing systematically with increasing temperature. Dames and Moore (1978) also indicated that for the typical shale, thermal conductivity measured perpendicular to the bedding is only about 75 percent of that measured parallel to the bedding. The anisotropy is an important feature of bedded sedimentary deposits, particularly shales.

Sandstone units in the reference repository would have higher average thermal conductivities than shales, although the data in Table 2.7 show an overlap of ranges for the two lithologies.

Heat capacity of "typical" shale was assigned values of 0.80 and 0.88 kJ/kg^{o}C between 0^{o} and 200^{o}C, respectively (Dames and Moore, 1978). Limited data for sandstones elsewhere suggest values of 0.77 and 0.97 kJ/kg^{o}C between 65^{o} and 200^{o}C would be appropriate for sandstones in the reference system.

Thermal expansion of shales during thermal loading is poorly quantified and will require considerable additional research and experimentation in the future. Recent experimental studies (Lappin and Olsson, in press) have suggested that the quantity of smectite or mixed-layer illite-smectite in a shale is the most important factor controlling shale response to heating. Lappin and Olsson have shown that shales containing even a small amount of smectite

can be subjected to dehydration and thus contraction during heating to 100°C. If the shales of the reference system, which contain approximately the same mineral constituents as the Pierre Shale, behave as the Pierre does during heating, then the host shales in the reference system might undergo a 2.2 ± 0.3 percent linear contraction upon heating to 100°C. This behavior inside the 100°C isotherm in the vicinity of the depository will probably alter the thermal, hydrologic, mechanical, and geochemical properties to some degree. Opening of fractures, new or preexisting, will decrease thermal conductivity and strength, and increase porosity and hydraulic conductivity. In areas where temperatures exceed 100°C, shales might be expected to again exhibit thermal expansion. Dames and Moore (1978) suggested coefficients of linear thermal expansion of 8.10×10^{-6} and 1.62×10^{-5} $^{\circ}C^{-1}$ for horizontal and vertical directions, respectively, in the "generic" shale. We have no basis for altering these values or suggesting a range of possible values.

Sandstones, except where they contain substantial amounts of clay, should display expansive behavior upon heating, and should expand in essentially an isotropic fashion. Skinner (1966) reported an average linear expansion coefficient of $1.0 \pm 0.2 \times 10^{-5}$ $^{\circ}C^{-1}$ for ten sandstone samples. This range of values can be used for sandstone units in the reference repository.

3.3.4 *Mechanical Properties*

Values for mechanical properties of geologic units in the reference repository system are not known directly and must be obtained from a compilation of data for geologic units outside the western Canada sedimentary basin. Dames and Moore (1978) compiled the data then available for the mechanical properties of shale and presented a tabular synthesis of the data into ranges of values (Table 3.3). The wide ranges given in Table 3.3 encompass the mechanical behavior of most shales. These ranges could be used for shales in the reference system, but they do not represent a realistic approximation of the properties of shales in the western Canada sedimentary basin or in any single shale deposit. The host shales of the reference repository could be expected to have mechanical properties that fall within a much narrower range. The Pierre Shale is the best mineralogic, lithologic, and stratigraphic correlative of the host shales for which a reasonable amount of data exists to quantify mechanical behavior. These data have been discussed in section 2.3.3.4 and are given in Table 2.6. Use of the values in Table 2.6 for average mechanical properties of the shales of the reference repository is suggested; however, the values given in Table 3.3 can provide broader limits should analysis of a larger range of shale properties be desirable.

Table 3.3 Range of values for mechanical properties of intact shale (after Dames and Moore, 1978).

Type of Property	Parameter	Range
Index	Bulk Density	1.9 - 3.0 gm/cm^3
	Natural Moisture Content	0 - 38%
	Porosity	0 - 45%
Mechanical	Young's Modulus	13.8 - 44130 MPa
	Poisson's Ratio	0.03 - 0.50
	Cohesion (10 to 24 MPa range)	0 - 29.3 MPa
	Friction Angle (10 to 24 MPa range)	4.2 - 56°
	Compressive Strength	0.5 - 255 MPa
	Tensile Strength	0 - 10.6 MPa

Several observations should be made regarding the mechanical properties of shale.

1. Shales generally display anisotropic mechanical behavior, with most mechanical properties having higher values parallel to the layering.

2. The changes in mechanical properties that might be induced by thermal loading are incompletely known.

3. Stress relief and exposure of high smectite shales to excess moisture might produce swelling and large decreases in strength.

4. Mechanical properties of the rock mass could be significantly affected by the presence of fractures.

Sandstone units in the sequence in the reference repository are assigned mechanical properties based on a review of available data for sandstones outside the principal study area. These values, given in Section 3.4, should bound within reasonable limits the mechanical behavior of sandstones in the reference system.

3.4 Summary of Selected Properties and Characteristics for the Reference Repository System in Shale

Section 3 has been devoted to the description of the reference repository system in shale. The aim of this effort has been to define, to the highest degree possible, recognizing the substantial gaps in the data base, the properties and characteristics of a real geologic system--viz., the western Canada sedimentary basin in southeastern Alberta, Canada. The reference repository, thus defined, is not the representation of the "average" of values and characteristics for shale systems in general; it is the representation of an existing natural system in shale with its own unique combination of geometry, properties, and boundary conditions. The western Canada basin was selected as a model for the reference system on the basis of data availability and the presence of thick shale units within the system. The process of characterization of the selected natural system and the subsequent definition of the reference system based on it does not necessarily identify an "ideal" shale system; rather, this effort has produced a hypothetical reference system, with the important characteristics of a typical real shale system, on which the risk assessment methodology can be exercised.

Table 3.4 presents a brief description of the host unit in the reference repository system. Properties of the principal units in the reference system are summarized in Table 3.5.

Table 3.4 Description and setting of the shale host rock in the reference repository system.

Lithology: Thick sequence of relatively uniform dark gray marine shale with occasional bentonite horizons; 50 to 75 percent smaller than 4 μm clay and 25 to 50 percent 4 to 62 μm silt: 300 to 400 m thick.

Mineralogy: 40 to 70 percent clay minerals; 20 to 40 percent quartz; 5 percent feldspar; small amounts of calcite, dolomite, biotite, pyrite, and organic material. Clay minerals: 35 percent smectite, 40 percent mixed-layer illite-smectite, 15 percent illite, 5 percent kaolinite, 5 percent chlorite.

Trace Elements: Uranium, 4 to 12 ppm; Strontium, 115 to 620 ppm.

Major Structures: Gently tilted strata dipping northward at about 5.5 m/km; minor faulting and shearing may be present locally along minor anticlinal and synclinal structures superimposed on the regional dip; individual faults are tight and may contain secondary mineralization, mostly calcite.

Jointing: Two major systems of near vertical joints, each with two orthogonal sets; principal system has sets oriented NW-SE and NE-SW; secondary system has sets oriented NS and EW; NE-SW set is usually dominant with joints of other sets often terminating against it. Third system comprised of horizontal bedding plane fractures.

State of Stress: Maximum principal stress vertical and equal to overburden pressure; intermediate principal stress horizontal, oriented NE-SW; minimum principal stress horizontal, oriented NW-SE.

Geothermal Gradient: 31^{o} to 33^{o}C/km (mean annual surface temperature, 5^{o}C).

Table 3.5 Summary of selected properties of geologic units in the reference repository system.

Unit	Lithology	Bulk Density (gm/cm^3)	Porosity (%)	Moisture Content (%)	Hydraulic Conductivity (cm/sec)	CEC[1] meq/100g)	Thermal Conductivity (J/M sec°C)
6	Shale	2.0-2.3	15-30	8-21	v.$1.0x10^{-6}$ - $1.0x10^{-10}$ h.$1.0x10^{-6}$ - $1.0x10^{-9}$	10-100	v.0.75 - 1.88@20°C h.1.00 - 2.50@20°C
5	Sandstone	2.2-2.4	15-20	7-11	v.$1.0x10^{-2}$ - $1.0x10^{-9}$ h.$1.0x10^{-2}$ - $1.0x10^{-8}$	5- 50	1.00 - 5.00@20°C
4	Shale	2.0-2.3	15-30	8-21	v.$1.0x10^{-6}$ - $1.0x10^{-10}$ h.$1.0x10^{-6}$ - $1.0x10^{-9}$	10-100	v.0.75 - 1.88@20°C h.1.00 - 2.50@20°C
3	Sandstone	2.2-2.4	15-20	7-11	v.$1.0x10^{-3}$ - $1.0x10^{-7}$ h.$1.0x10^{-3}$ - $1.0x10^{-6}$	5- 50	1.00 - 5.00@20°C
2	Sandstone	2.2-2.4	15-20	7-11	v.$1.0x10^{-3}$ - $1.0x10^{-7}$ h.$1.0x10^{-3}$ - $1.0x10^{-6}$	5- 50	1.30 - 6.40@20°C
1	Sandstone	2.2-2.4	15-20	7-11	v.$1.0x10^{-4}$ - $1.0x10^{-6}$ h.$1.0x10^{-4}$ - $1.0x10^{-5}$	5- 50	1.30 - 6.40@20°C

[1]Cation Exchange Capacity

Table 3.5 Continued

Unit	Heat Capacity (kJ/kg°C)	Coefficient of Linear Thermal Expansion ($°C^{-1}$)	Young's Modulus (MPa)	Poisson's Ratio	Compressive Strength (MPa)	Tensile Strength (MPa)
6	0.80@0°C 0.88@200°C	Same as Unit 4	v.483 h.965	0.2	See Figures 2.13 and 2.14	v.0.17 h.0.34
5	0.77@65°C 0.97@200°C	0.80×10^{-5} to 1.20×10^{-5}	5000 to 20,000	0.2	25 to 75	1.25 to 3.75
4	0.80@0°C 0.88@200°C	v. -0.022 ± 0.003 0 to 100°C, 1.62×10^{-5} above 100°C h. -0.022 ± 0.003 0 to 100°C, 8.10×10^{-6} above 100°C	v.483 h.965	0.2	See Figures 2.13 and 2.14	v.0.17 h.0.34
3	0.77@65°C 0.97@200°C	0.80×10^{-5} to 1.20×10^{-5}	5000 to 20,000	0.2	25 to 75	1.25 to 3.75
2	0.77@65°C 0.97@200°C	0.80×10^{-5} to 1.20×10^{-5}	5000 to 20,000	0.2	25 to 75	1.25 to 3.75
1	0.77@65°C 0.97@200°C	0.80×10^{-5} to 1.20×10^{-5}	5000 to 20,000	0.2	25 to 75	1.25 to 3.75

4. THE GROUND-WATER FLOW REGIME AND CONTAMINANT TRANSPORT

The results of simulations of ground-water flow and contaminant transport are presented in this section. The multidimensional simulations all involve the DPCT model (Schwartz and Donath, 1980). This model differs from more conventional ones in that the movement of contaminants is simulated using a hybrid deterministic-probabilistic technique which does not involve a direct solution of the transport equation (Schwartz and Crowe, 1980). Ground-water seepage velocities are calculated at node points within the flow domain from a knowledge of hydraulic head, porosity, and hydraulic conductivity values. Hydraulic heads are determined numerically by solving the boundary value problem for flow. Moving reference particles, tagged with a specified quantity of mass, are introduced to the region at the contaminant source(s). These particles are moved with both deterministic and random components of motion. The deterministic component is controlled by the ground-water seepage velocity, whereas the random component is controlled by the dispersive character of the porous media. The simulation proceeds by allowing the reference particles to move through the domain subject to conditions along the boundary. Concentrations of a component of interest are simply a function of the density of reference particles within the region. Readers can refer to Schwartz and Crowe (1980) for discussion of the basic theory, a detailed description and listing of the computer code, and input data for several sample problems; the reader is referred to Schwartz and Donath (1980) for applications of the flow and transport model to scenario evaluation.

The size of the region representing the reference system for shale and the relatively complex pattern of layering within it has necessitated the use of a very large grid system. The large number of nodes coupled with the large number of constant head nodes requires the optimization of array storage in the DPCT code and the partitioning of one extremely large array. In addition, it was necessary to generalize possible configurations of the bottom boundary. These requirements led to some modification of the basic DPCT code for the present study.

All the data required for the simulation of the reference repository system for shale are tabulated in the Appendix. These data coupled with discussions in the previous section should make it possible to reproduce the reference system simulations using other computer models. The hydrologic and transport properties used for geologic units in the preliminary model simulations are given in Table 4.1. As an initial estimate, we have assumed that the vertical component of hydraulic conductivity is 20 percent of the horizontal compo-

Table 4.1 Hydrologic and transport properties assigned geologic units in preliminary model runs.

	Hydraulic Conductivity (cm/sec)		Porosity (%)	Dispersion Length (m)
Unit 6	Vert.	$1x10^{-6}$ to $1x10^{-8}$	15	3.0
	Horiz.	$5x10^{-6}$ to $5x10^{-8}$		
Unit 5	Vert.	$1x10^{-3}$ to $1x10^{-8}$	15	3.0
	Horiz.	$5x10^{-3}$ to $5x10^{-8}$		
Unit 4	Vert.	$1x10^{-8}$	15	3.0
	Horiz.	$5x10^{-8}$		
Unit 3	Vert.	$1x10^{-4}$ to $1x10^{-6}$	15	3.0
	Horiz.	$5x10^{-4}$ to $5x10^{-6}$		
Unit 2	Vert.	$1x10^{-4}$ to $1x10^{-6}$	15	3.0
	Horiz.	$5x10^{-4}$ to $5x10^{-6}$		
Unit 1	Vert.	$1x10^{-5}$	15	3.0
	Horiz.	$5x10^{-5}$		

nent for all units. In addition, we have assigned a constant porosity across the entire flow domain. This considerably simplifies the modeling problem and is justified because the time to exit the host unit was the only transport characteristic examined in these preliminary runs.

The results presented consist of simulations of the steady state pattern of ground-water flow along the reference section, and of the spread of contaminant away from a depository located in Unit 4 (Figure 3.1B). One can obtain a qualitative understanding of ground-water flow conditions in the domain by examining the equipotential lines depicted in the lowest section of Figure 4.1. The variation in hydraulic conductivity in the vertical and horizontal directions, respectively, is depicted in the upper two sections of Figure 4.1. For the transport simulations, contaminant sources representing the repositories are located at two places in Unit 4. In both cases, they are located toward the south end of the domain to take advantage of the downward flow conditions that exist beneath the permeable part of the Milk River Formation (represented as Unit 5).

Detailed examination of the equipotential lines shows the important controls on flow that are exerted by the highly permeable portions of Unit 5 (Figure 4.1; see also Figure 3.1). In the southern part of the domain (right-hand side of section), high hydraulic heads within Unit 5 force water to move out of the unit along both the top and bottom contacts. Artesian heads, which are simulated in Unit 5, are sufficient to produce flowing wells. Such a condition is representative of the actual situation where many of the wells completed in the Milk River Formation are now or were flowing. Along the northern half of the reference section (left side), the principal direction of ground-water flow is upward (Figure 4.1). Although we have no direct way to verify the degree to which this condition of flow is representative of the natural system, this situation does provide an explanation as to why the δO and D content of water from the Milk River Formation resembles that of the underlying Bow Island Formation. Thus, the simulation is fully consistent with available field observations. As has been our experience with the reference system for bedded salt (Schwartz and Donath, 1980), flow in the more permeable units such as the Milk River or Bow Island Formations (represented in the reference section as Units 5 and 3) tends to be dominantly lateral. Flow in the less permeable units tends to be dominantly vertical.

As a direct result of the modeling, values of seepage velocity are calculated at a large number of points across the flow domain. Options in the DPCT code allow these data to be listed. Because there can be marked variability in

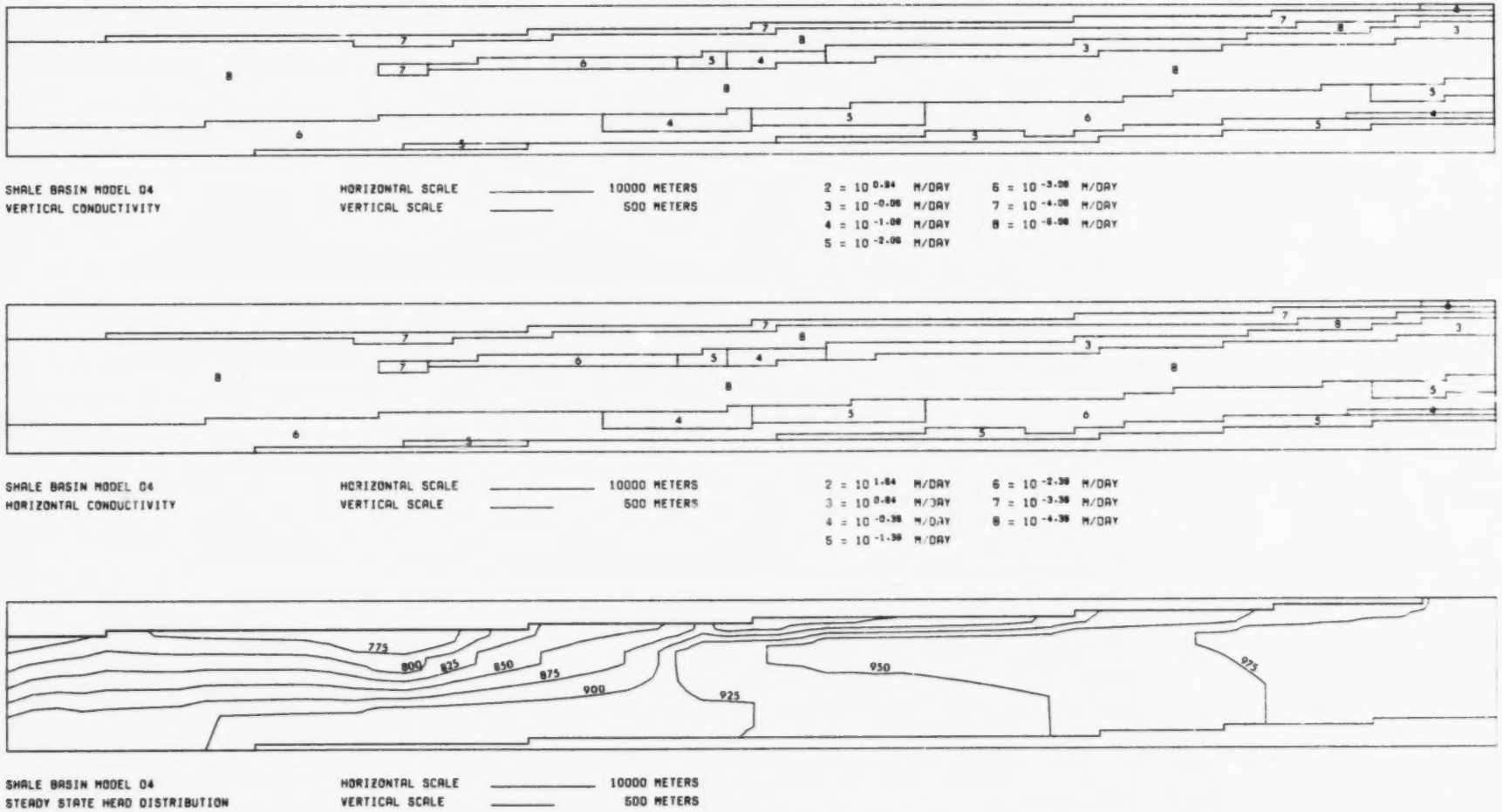


Figure 4.1 Cross sections showing values used for vertical and horizontal hydraulic conductivities (upper two sections) and equipotential contours of hydraulic head (lower section) in the reference repository system.

hydraulic gradients within a single unit, velocities can also be quite variable. For example, within the disposal unit (Unit 4), velocities range from a maximum of 1×10^{-5} m/day to a minimum of 1×10^{-6} m/day with most of the values falling toward the lower end of the range. In the most permeable parts of Unit 5, seepage velocities are approximately 2×10^{-2} m/day. The value for Unit 3 is 2×10^{-5} m/day.

Because the source locations are toward the south end of the flow domain, contaminants entering the ground-water system will be carried downward, resulting in a longer residence time in the flow system. It is assumed for purposes of modeling that contaminants enter the flow system at a constant rate. For these simulations, 100 particles were added at the beginning of each time step and, typically, 20 time steps of 20,000 years each were utilized. Specifications of such a simple loading function is a matter of convenience only. The DPCT code has the flexibility to approximate any complex function for loading.

Figure 4.2 depicts the pattern of contaminant spread from a line source across the midline of the cell which has its lower left corner at row 14 and column 40. The values shown on the figure are relative concentrations. As anticipated, the contaminants move generally downward; they remain confined in the host unit for times up to 135,000 years, in spite of appreciable spreading from the source. Very similar results are obtained for a depository located near row 16 and column 51 (Figure 4.3). However, in this case the rate of spreading is much lower because of decreased hydraulic gradients at this point in the flow domain. Both of the transport simulations included here indicate that, for the conditions which we have considered, contaminant confinement far in excess of 100,000 years is possible in this reference repository system. It should be noted, also, that the transport simulations presented do not incorporate the effects of sorption or other retardation factors that would need to be considered in the evaluation of a site for repository development. The primary objective in this study is to define a representative system adequately enough to permit its transport characteristics to be evaluated in both normal and disrupted states for a representative range of values of all important transport parameters.

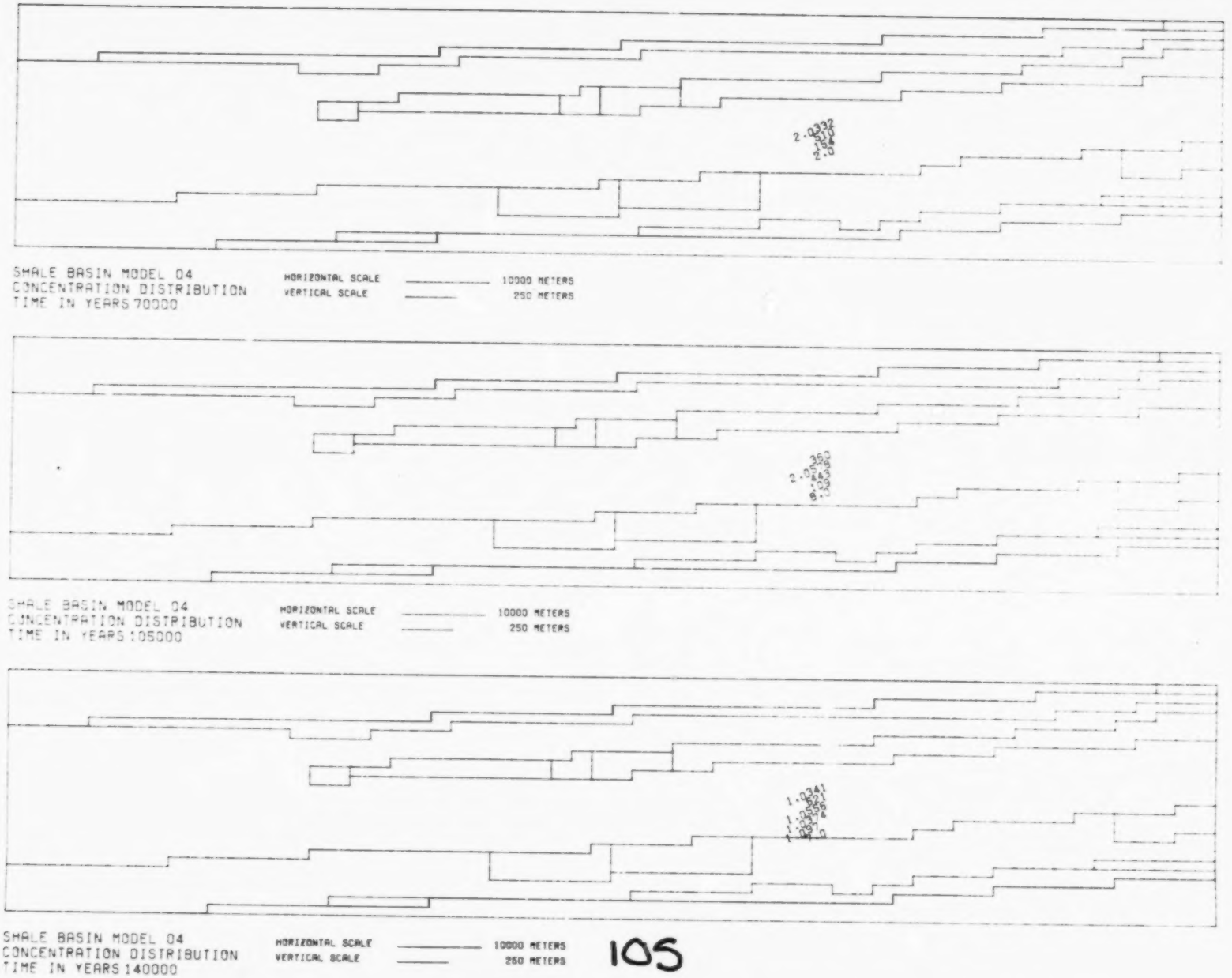


Figure 4.2 Cross sections showing contaminant concentration distributions from a source in row 14, column 40, of the reference repository system.

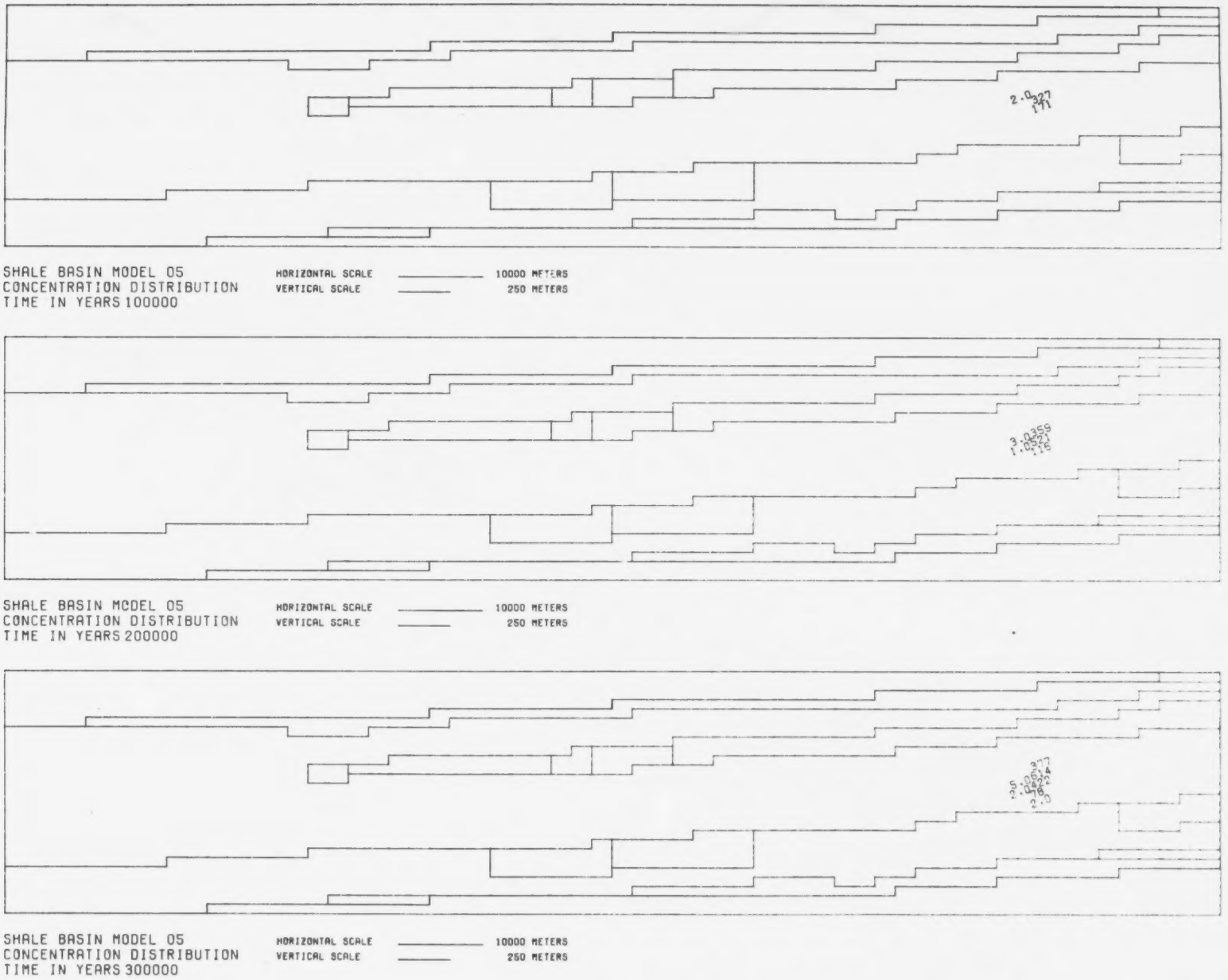


Figure 4.3 Cross sections showing contaminant concentration distributions from a source in row 16, column 51, of the reference repository system.

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5. GEOLOGIC PROCESSES AND EVENTS INFLUENCING REPOSITORY SYSTEM RESPONSE

Geologic systems are dynamic systems undergoing constant natural evolution. They are affected by a variety of natural processes that act over long periods of geologic time. Natural events, occurrences of shorter duration, affect the system at different times during its existence. The key to the identification of those natural processes and events that will influence a particular repository system is a knowledge of the history of that system during the geologic past. Estimation of probable process rates and event recurrence intervals is most confidently made through extrapolation from the geologic record. In addition to the evolution of the geologic system in response to natural processes and events, substantial alteration of natural conditions will be induced by excavation of the depository and by waste emplacement. These effects must be evaluated in the context of the dynamic natural system in which they occur. The current methodology for assessment of risk associated with disposal of radioactive wastes in geologic media involves analysis of a combination of circumstances (a scenario) that might lead to release of contaminants to the biosphere. The most important step in such an approach is a complete list of plausible scenarios. Section 5 of this report provides a preliminary discussion of natural geologic processes and events that might influence the capability of the reference repository system to isolate contaminants from the biosphere and that should be accounted for in scenario analysis.

5.1 Tectonic and Seismic Activity

Tectonic processes can have widespread regional effects or localized effects. Large-scale uplift, subsidence, or tilt of the repository system might substantially alter boundary conditions of the ground-water flow system, the state of stress in the geologic media, or the rates of other processes such as erosion or sedimentation. Local faulting anywhere in the repository system could disrupt the natural ground-water potential field and change the direction and velocity of flow through the disposal medium.

With some notable exceptions, shale systems in North America occur within some of the most tectonically stable parts of the continent. The three large systems studied for this report have not been subjected to large-scale tectonism for tens of millions of years. Over the next million years, regional uplift, tilting or subsidence of any significance is unlikely for these systems. However, scenario analyses should evaluate tectonic processes and their

effects (e.g., faults) in order to determine the sensitivity of the reference system to large scale tectonism.

All three of the studied basins have been subjected to minor faulting during the past million years. Neither the scale nor the frequency of recent faulting is known in any detail. The occurrence of faulting in the repository system is likely to have considerable influence on ground-water flow and, as such, requires detailed treatment in scenario analyses. Recent study of the problem of faulting in a repository system (Donath and Cranwell, 1980) has presented methods for determining the probability that an undetected fault might exist in a repository system, and for determining the probability that a fault might develop or that movement along an existing fault might occur. The previously cited study by Schwartz and Donath (1980) evaluates the effects on ground-water flow and transport of a fault in the reference repository system in bedded salt, and provides insights into the general effects that might be expected in other systems.

Most large sedimentary basins in North America are located in seismically stable areas. The Illinois Basin, however, stands as an example of a shale system with a moderate level of seismic activity. The probability of recurrence of a very large magnitude seismic event in the Illinois Basin is considered high because of the proximity to the epicenter of the 1811-1812 New Madrid quakes, the largest historic quakes in the continental United States. The length of historic observation of seismic activity is much too short to estimate recurrence rates for most seismic events in North America. Thus, the occurrence of large seismic events over the life of a repository is possible and should be considered likely.

Recently, numerical models have been used to simulate the effects of seismic events on a repository system (Pratt et al., 1979; Wahi et al., 1980). In general these studies show that moderate earthquakes do not cause instability of excavations or major fracturing of the rock mass. Damage to underground openings is significantly less than damage at the surface for the same size earthquake. The severity of underground effects are related to mechanical properties of the geologic media and to the intensity of the seismic acceleration. Effects should be reduced after openings are backfilled.

5.2 Igneous Activity

Igneous activity is rare within continental shale basins such as those studied for this report. There is no evidence for igneous intrusion in the interiors of any of the three systems, but intrusives are present in the peripheral areas of all three. We feel that candidate repository sites in shale can be selected in regions where the likelihood of future igneous intrusion is negligible. Nevertheless, scenario analyses of the bedded salt reference repository system have determined that the effects of the presence of an extremely low permeability barrier, such as an igneous dike, are sufficently significant that igneous processes or features should be considered in the risk assessment methodology.

5.3 Subsurface Geochemical Processes

Subsurface geochemical processes that might influence the performance of a repository system include: changes in ground-water chemistry, dissolution of the geologic media, precipitation or cementation, and alteration of sorption capacity of the geologic media.

Changes in ground-water chemistry from that present at the time of site characterization can be part of the normal evolution of the ground-water system, as with the flushing of connate waters by meteoric waters in the three basins studied for this report. Changes in chemistry can also result as a consequence of alterations in flow rates, flow directions, or thermal load. A change in chemical composition of the ground water might alter the rate of dissolution of the waste and thus influence contaminant transport. Variations in ground water chemistry can also initiate changes in dissolution of the geologic media, in precipitation or cementation, or in sorption capacity of the media.

The host rock in a shale depository is essentially insoluble in comparison to other beds, particularly evaporites such as gypsum, anhydrite, and bedded salt. In the southern part of the Williston Basin, evaporite dissolution and collapse of overlying strata have produced very large breccia pipes (Gott et al., 1974). One such pipe that originates in the Minnelusa Formation is known to penetrate 396 m (1300 ft) of the overlying section. These features in South Dakota are probably major conduits for upward leakage of ground water from deep to shallow aquifers. The severity of the consequences of such a disruption on the reference system probably justifies its treatment in scenario analyses.

Precipitation and cementation tend to act as sealants in the system by closing off porosity and decreasing permeability. Such processes can either enhance or degrade the waste isolation capability of a repository system, depending on where and to what extent they occur. Schwartz and Donath (1980) evaluated the effects of regions of altered hydraulic conductivity on the transport of contaminants in the ground-water system of the reference repository system in bedded salt. Their methods can be applied to the effects of several processes--such as faulting, igneous intrusion, cementation, or dissolution--that alter the hydraulic properties of the geologic media. At present there is no information on the rates at which cementation or dissolution processes might proceed in the repository system.

Changes in the exchange capacity of clay minerals in the geologic media can enhance or severely reduce the capacity of the system to retard radionuclides from transport in ground water. The ion exchange capacity of a clay mineral depends on the availability of exchange sites. Saturation of these sites with stable ions in ground water restricts the ability of the clay to absorb additional ions. Any scenario that alters the ground-water flow system might also alter the chemistry of ground water and the sorption capacity of media in large parts of the system.

5.4 Surface Geological Processes

The list of possible surface processes that might affect a repository system is large. Of these, four--climatic change, erosion, deposition, and glaciation--have during the past one million years or so produced large changes in each of the three geologic systems studied for this report.

The radical and cyclic extremes of past climatic fluctuations have produced, at times, continental glaciation and, at times, climates like the present. Most climatologists agree that the climatic cyclicity will continue, probably with the average 100,000 year periodicity typical of the past two million years. Because the Earth is now within one of these cycles, it is highly likely that during the next 100,000 years any repository system will be subjected to extreme variation in surface temperature, precipitation, and evapotranspiration. These effects could be incorporated into scenario analysis with appropriate changes in boundary conditions of the ground water model.

During the Quaternary the western Canada sedimentary basin in the study region was repeatedly covered by glacial ice. The maximum extent of glaciation was about 100 km south of the southern boundary of the reference cross section.

Scenario analyses should include repeated glaciation covering at various times all or part of the reference system.

Glacial drift in the reference repository is about 100 m thick. This gives an approximate value for the amount of deposition that glaciation could produce in the reference system over the next one million years.

Erosion to any significant depth is probably unlikely in the reference system as defined. There is little surface relief, few rivers, and very low rainfall. Certainly some shale systems might be much more susceptible to erosion. Shale is one of the most easily eroded types of rock. Local erosion to depths of about 100 m below the present surface configuration could be incorporated into a plausible scenario package.

6. NONGEOLOGIC PROCESSES AND EVENTS INFLUENCING REPOSITORY SYSTEM RESPONSE

As stated in the preceding discussion, the natural geologic system in which radioactive waste is emplaced has a history and a potential for natural evolution under the influence of a variety of natural processes and events. One very real challenge faced by those who wish to determine system response to waste emplacement is the present shortfall in knowledge of interactions between natural processes and processes or events initiated by the placement of waste in the system. Additional problems in the prediction of future changes in a repository system arise from the unpredictability of human acts. The following is a preliminary discussion of nongeologic processes and events that should be incorporated into scenario analyses of the reference reposity in shale.

6.1 Construction-Related Factors

The excavation of large scale caverns necessary for radioactive waste emplacement constitutes a major disruption of the natural system. For successful waste isolation, possible adverse effects of excavation must be minimized. Scenario analyses should account for a wide range of possible excavation-related effects such as (1) mine pillar or roof collapse with subsequent disruption of overlying strata, (2) degradation of mechanical integrity and hydrologic properties of shales in the vicinity of the excavation caused by dessication or by moisture sorption, and (3) leakage of seals around shafts or boreholes. Mine pillar or roof collapse during the operational period of the depository could affect a large region in the vicinity of the depository excavation. The larger the mine area affected, the larger the potential effect on overlying strata and surface structures. Moisture change in near-field shales could have some localized adverse influences on opening stability which might contribute ultimately to larger failures. Leakage around seals in shafts and boreholes must be assumed during the life of the depository, and designs must be created to minimize so-called "U-tube" effects.

6.2 The Induced Thermal Load

The alteration of the properties of shale caused by high temperatures related to the emplacement of hot waste could have potentially severe influences on the repository system. These effects are probably the most difficult to

assess because of current lack of understanding of thermal properties of shales. To incorporate the full range of possible shale behavior, scenario analyses should consider cases at one extreme for which the thermal load causes substantial contraction of shales in the near field and, at the other extreme, for which it causes only expansion. In either case, volume changes are likely to be coupled with alterations in hydrologic properties. Contraction would be expected to cause some increase in porosity and in hydraulic conductivity. Expansion might result in decreased hydraulic conductivity near the depository because of fracture closure, but increased conductivity in overlying strata because of localized fracturing.

6.3 Exploration for Resources

Repository systems in shale and other geologic media should be selected so as to minimize the likelihood that they will be penetrated by boreholes drilled by future populations in search of natural resources. This can be accomplished by avoiding regions with geologic or hydrologic features that might be interpreted as having resource value. Regardless of the steps taken to minimize the probability of penetration, boreholes must be included in the list of plausible scenarios that should be evaluated.

7. PREFERENTIAL AND ADVERSE FEATURES AND CHARACTERISTICS OF SHALE AS A MEDIUM FOR ISOLATION OF RADIOACTIVE WASTES

This section discusses those features and characteristics of shales and of the geologic systems in which shales occur that can be considered either preferential or adverse in the evaluation of shales as a potential medium for radioactive waste isolation.

Shales are most abundant in large intracratonic basins that contain thick sequences of sedimentary strata. In these settings, shales are often thick, extensive, and uniform in their mineralogic and textural compositions. As such, they constitute one of the most extensive and uniform lithologies under consideration as a waste disposal medium.

Large-scale geologic systems in sedimentary basins are relatively well known from extensive exploration for natural resources. Exploratory programs have fostered the development of characterization tools and techniques, and models of depositional, diagenetic, tectonic, and hydrologic processes in order to sharpen predictive skills necessary for resource discovery and evaluation. Many of these predictive skills and the experience gained from years of application are directly suited to the evaluation of shale systems as waste disposal systems. It should be noted, however, that the association of shales with resource-bearing rocks will eliminate some areas from consideration for waste isolation, and future exploration for resources in sedimentary sequences could make very high the likelihood that any particular area will eventually be penetrated by a borehole.

Whereas the systems and, in particular, the reservoir rocks in those systems have received considerable attention in resource exploration programs, fine-grained low-permeability shales have received less study. Recently, large-scale programs to evaluate the resource potential of oil and gas in certain shales have developed the funding necessary to provide a rapid expansion of knowledge of shale deposits. However, like most candidate disposal media, shale will require extensive study before certain questions of suitability for waste isolation can be specifically answered.

The low intergranular permeability and generally low fracture permeability of shales is well known. However, techniques for in situ measurement of hydrologic properties of shales and for surveying fracture spacing, orientation, aperture, and continuity are poorly developed.

The clay mineral content of shales gives them potentially excellent sorptive qualities. Laboratory analyses that are aimed at quantifying such parameters as the distribution coefficient fall far short of applicability to specific shales in specific field situations. Of particular concern is the influence of ground-water chemistry on sorptive capacity of shale. Many shales contain concentrated brines whose dissolved stable species offer substantial competition for exchange sites on clays and sesquioxides. In addition, organic matter, ubiquitous in shales, might either enhance or retard the migration of specific nuclides. These effects need quantification in tests that reproduce natural conditions. Once techniques are developed to assess the mineralogic, geochemical, and sorptive characteristics of a particular shale at a site, extrapolation of those characteristics away from the immediate vicinity of the site will be facilitated by the lateral uniformity of the medium.

The mechanical characteristics of shale deposits might have both potentially favorable and unfavorable impacts on the construction, operation, and evaluation of a radioactive waste depository. Recognizing the broad range of behavior that shales can display under applied mechanical loads, we can still make some generalizations about shales. In general, shales display elasto-plastic behavior. Minor ductile deformation in the depository proximity might limit propagation of existing fractures and inhibit formation of new fractures under altered stress conditions caused first by excavation and then by thermal loading. But, such potential for plastic deformation will also likely require design of a more extensive excavation support system than required in some other rock types. Any support system in shale should be designed not only to enhance opening stability through stress redistribution, but should account for the particular susceptibility of shales to weathering and changing moisture conditions by maintaining natural moisture conditions in the near-field rocks. Because the mechanical properties of shales are very sensitive to changes of pore pressure, confining stress, and moisture content, programs to evaluate the properties of shales and other argillaceous sedimentary strata should pay particular attention to techniques of sample collection and handling. Every reasonable attempt should be made to minimize disturbance of the sample and, to the greatest extent possible, to preserve the moisture and stress conditions of the in situ environment.

The sensitivity of some shales, particularly those containing smectite clay minerals, to alteration under conditions of thermal loading bears emphasis in a discussion of features affecting suitability of shale as a medium for waste disposal. The behavior displayed by a specific shale when exposed to elevated temperatures depends to a large degree on the thermal history of that shale deposit. Undoubtedly, thick sequences of low smectite high temperature shales, such as the illitic Paleozoic shales of the Illinois and Appalachian Basins, would be less susceptible to dehydration and mineral alteration than the low temperature smectite shales of the Cretaceous of the Great Plains. However, present information and current testing programs are insufficient to adequately quantify the range of behavior that should be expected from shales of varying mineralogies and thermal histories.

In conclusion, the present state of knowledge of the characteristics of shales and the behavior of shales in the presence of radioactive wastes does not identify any feature or group of features of shales that make them unworthy of further consideration as a radioactive waste disposal medium.

REFERENCES

Abel, J. F., and D. W. Gentry, 1975, Evaluation of excavation experience: Pierre Shale: ORNL/SUB-75/70347, 108 pp.

Alberta Society of Petroleum Geologists, 1960, Lexicon of Geologic Names in the Western Canada Sedimentary Basin and Arctic Archipelago, 596 pp.

Alberta Society of Petroleum Geologists, 1966, Geological History of Western Canada: McGrossan, R. G. (editor), 230 pp.

Armon, W. J., and O. W. Rees, 1960, Chemical evaluation of Illinois oil shales: Illinois Geol. Survey Circ. 307, 22 pp.

Babcock, E. A., 1974, Jointing in southern Alberta: Canadian Jour. Earth Sci., v. 11, p. 1181-1186.

Babcock, E. A., 1978, Measurement of subsurface fractures from dipmeter logs: Am. Assoc. Petroleum Geologists Bull., v. 62, no. 7, p. 1111-1126.

Barrows, M. H., R. M. Cluff, and R. D. Harvey, 1979, Petrology and maturation of dispersed organic matter in the New Albany Shale Group of the Illinois Basin: U.S. Dept. of Energy, METC/SP-79/6, p. 85-114.

Baxter, J. W., and G. A. Desborough, 1965, Areal geology of the Illinois fluorspar district, Pt. 2--Karbers Ridge and Rosiclare Quadrangles: Illinois Geol. Survey Circ. 385, 40 pp.

Bell, A. H., Elwood Atherton, T. C. Buschbach, and D. H. Swann, 1964, Deep oil possibilities of the Illinois Basin: Illinois Geol. Survey Circ. 368, 38 pp.

Bergstrom, R. E., 1968, Feasibility of subsurface disposal of industrial wastes in Illinois: Illinois Geol. Survey Circ. 426, 18 pp.

Birch, F., J. F. Schairer, and H. C. Spicer, 1942, Handbook of physical constants: Geological Soc. of America Special Paper no. 36, 325 pp.

Blixt, J. E., 1941, Cutbank oil and gas field, Glacier County, Montana, in Levorsen, A. I. (editor), Stratigraphic type oil fields: Am. Assoc. Petroleum Geologists, p. 327-381.

Black, H. N., H. E. Ripley, and W. H. Beecroft, 1980, Fracturing fluid improvements for gas wells in Canada: Jour. Can. Petrol. Tech., April-June, p. 58-64.

Bond, D. C., 1972, Hydrodynamics in deep aquifers of the Illinois Basin: Illinois Geol. Survey Circ. 470, 72 pp.

Bredehoeft, J. D., C. R. Blyth, W. A. White, and G. B. Maxey, 1963, Possible mechanisms for concentration of brines in subsurface formations: Am. Assoc. Petroleum Geologists Bull., v. 47, no. 2, p. 257-269.

Bredehoeft, J. D., and G. F. Pinder, 1973, Mass transport in flowing ground water: Water Resour. Res., v. 9, no. 1, p. 194-221.

Brown, C. B., 1944, Report on an investigation of water losses in streams flowing east out of the Black Hills, South Dakota: U.S. Department of Agriculture, Soil Conservation Service, Special Report 8, 45 pp.

Buschbach, T. C., and G. E. Heim, 1972, Preliminary geologic investigations of rock tunnel sites for flood and pollution control in the Greater Chicago Area: Illinois Geol. Survey Environmental Geology Note 52, 35 pp.

California Department of Water Resources, 1971, Sea water intrusion: Aquitards in the coastal groundwater basin of Oxnard plain, Ventura County: Bull. 63-4, 569 pp.

Carrigy, M. A., and G. B. Mellon, 1964, Authigenic clay mineral cements in Cretaceous and Tertiary sandstones Alberta: Jour. of Sed. Pet., v. 34, no. 3, p. 461-472.

Cartwright, K., 1970, Ground-water discharge in the Illinois Basin as suggested by temperature anomalies: Water Resour. Res., v. 6, no. 3, p. 912-918.

Clayton, R. N., I. Friedman, D. L. Graf, T. K. Mayeda, W. F. Meents, and N. F. Shimp, 1966, The origin of saline formation waters: Jour. Geophysical Res., v. 71, no. 16, p. 3869-3882.

Crandell, D. R., 1950, Revision of Pierre Shale of central South Dakota: Am. Assoc. Petroleum Geologists Bull., v. 34, no. 12, p. 2337-2346.

Crandell, D. R., 1958, Geology of the Pierre area, South Dakota: U.S. Geol. Survey Prof. Paper 307, 83 pp.

Culver, G. E., 1890, The problem of irrigation in the Dakotas: State Univ. of South Dakota, Bull. no. 1, 7 pp.

Dames and Moore, 1978, Technical support for GEIS: Radioactive waste isolation in geologic formations: U.S. Dept. of Energy, Y/OWI/TM-36, v. 7, 137 pp.

Darton, N. H., 1909, Geology and underground waters of South Dakota: U.S. Geol. Survey Water-Supply Paper 227, 156 pp.

Davis, S. N., 1969, Porosity and permeability of natural materials, in DeWiest, R. J. M. (editor), Flow Through Porous Media: Academic Press, New York, p. 54-89.

DOE, 1978, Eastern Gas Shales Project Annual Report Fiscal Year 1977: U.S. Dept. of Energy, MERC/CR-78/5, 160 pp.

Donath, F. A., and R. M. Cranwell, 1980, Probability of faulting in a repository system: Final Report prepared for Sandia National Laboratories under contract no. 46-1580, CGS/SL80F090, 35 pp.

Earlougher, R. C., Jr., 1977, Advances in well test analysis: Society of Petroleum Engineers of AIME, Monograph Volume 5, 264 pp.

Emrich, G. H., and R. E. Bergstrom, 1962, Des Plaines Disturbance, northeastern Illinois: Geol. Soc. of America Bull., v. 73, p. 959-968.

Freeze, R. A., and J. A. Cherry, 1979, Groundwater: Prentice-Hall Inc., New Jersey, 604 pp.

Garland, G. D., and D. H. Lennox, 1962, Heat flow in western Canada: The Geophysical Jour. of the Royal Astro. Soc., v. 6, p. 245-262.

Glaister, R. P., 1958, Lower Cretaceous of southern Alberta and adjoining areas. Am. Assoc. Petroleum Geologists Bull., v. 43, no. 3, p. 590-640.

Gondouin, M., M. P. Tixie, and C. Scala, 1958, Streaming potential and the S. P. Log: Jour. Petrol. Tech., v. 10, no. 8, p. 170-179.

Gott, G. B., D. E. Wolcott, and C. G. Bowles, 1974, Stratigraphy of the Inyan Kara Group and localization of uranium deposits, southern Black Hills, South Dakota and Wyoming: U.S. Geol. Survey Prof. Paper 763, 57 pp.

Gries, J. P., 1942, Economic possibilities of the Pierre Shale: South Dakota Geol. Survey Report of Inv. no. 43, 79 pp.

Gries, J. P., 1954, Cretaceous rocks of Williston Basin: Am. Assoc. Petroleum Geologists Bull., v. 38, no. 4, p. 443-453.

Gries, J. P., P. H. Rahn, and R. K. Baker, 1976, A pump test in the Dakota Sandstone at Wall, South Dakota: South Dakota Geol. Survey Circ. 43, 2 pp.

Grim, R. E., W. F. Bradley, and W. A. White, 1957, Petrology of the Paleozoic shales of Illinois: Illinois Geol. Survey Report of Inv. 203, 35 pp.

Harvey, R. D., 1967, Thermal expansion of certain Illinois limestones and dolomites: Illinois Geol. Survey Circ. 415, 33 pp.

Harvey, R. D., W. A. White, R. M. Cluff, J. K. Frost, and P. B. DuMontelle, 1977, Petrology of the New Albany Shale Group (Upper Devonian and Kinderhookian) in the Illinois Basin: A preliminary report: U.S. Dept. of Energy, MERC/SP-77/5, p. 239-265.

Heigold, P. C., R. F. Mast, and K. Cartwright, 1971, Temperature distributions and ground-water movement associated with oil fields in the Fairfield Basin, Illinois, Proceedings of Symposium on Future Petroleum Potential of NPC Region 9 (Illinois Basin, Cincinnati Arch, and northern part of Mississippi Embayment), March 11-12, 1971: Illinois Geol. Survey Illinois Petroleum 95, p. 127-140.

Hilton, J., 1978, Wireline evaluation of the Devonian shale, a progress report: U.S. Dept. of Energy, MERC/SP-77/5, p. 68-79.

Hitchon, B., 1964, Formation fluids, Chapter 15 in Geological History of Western Canada: Alberta Soc. of Petroleum Geologists, Calgary, Alberta.

Hitchon, B., 1969a, Fluid flow in the western Canada sedimentary basin: 1. Effect of Topography: Water Resour. Res., v. 5, no. 1, p. 186-195.

Hitchon, B., 1969b, Fluid in the western Canada sedimentary basin: 2. Effect of Geology: Water Resour. Res., 5: no. 2, p. 460-469.

Hitchon, B., and I. Friedman, 1969, Geochemistry and origin of formation waters in the western Canada sedimentary basin: 1. Stable isotopes of hydrogen and oxygen: Geochim. Cosmochim. Acta., 33, p. 1321-1349.

Hoffman, J., and J. Hower, 1979, Clay mineral assemblages as low grade metamorphic geothermometers: Application to the thrust faulted disturbed belt of Montana, U.S.A: Soc. Econ. Petrologists and Mineralogists Special Pub. 26, p. 55-79.

Hughes, G. M., P. Kraatz, and R. A. Landon, 1966, Bedrock aquifers of northeastern Illinois: Illinois Geol. Survey Circ. 406, 15 pp.

Kalyoncu, R. S., W. G. Coppins, D. T. Hooie, and M. J. Snyder, 1978, Characterization and analysis of Devonian shales: 1. Physical characterization: U.S. Dept. of Energy, MERC/SP-77/5, p. 230-258.

Kemper, W. D., 1961, Movements of water as affected by free energy and pressure gradients: Soil Sci. Soc. of America Proc., v. 25, p. 255-265.

Kendall, A. C., and F. Simpson, 1974, Calcite layers in the uppermost Medicine Hat Sandstone (Upper Cretaceous) of southwestern Saskatchewan: Bull. of Can. Petroleum Geol., v. 22, no. 1, p. 34-41.

Kim, M. M., and H-Y. Ko, 1977, Multi-stage triaxial testing: Technical Report of Investigation, U.S. Bureau of Mines Grant No. G0155056.

Lamar, J. E., 1957, Chemical analyses of Illinois limestones and dolomites: Illinois Geol. Survey Report of Inv. 200, 33 pp.

Lappin, A. R., and W. A. Olsson, in press, Material properties of Eleana Argillite--extrapolation to other argillaceous rocks, and implications for waste management, U.S. Dept. of Energy.

Leventhal, J. S., and M. B. Goldhaber, 1978, New data for uranium, thorium, carbon and sulfur in Devonian black shale, from West Virginia, Kentucky, and New York: U.S. Dept. of Energy, MERC/SP-77/5, p. 259-296.

Lineback, J. A., 1966, Deep-water sediments adjacent to the Borden Siltstone (Mississippian) delta in southern Illinois: Illinois Geol. Survey Circ. 401, 48 pp.

Magara, K., 1976, Thickness of removed sedimentary rocks, paleopore pressure, and paleotemperature, southwest part of western Canada basin: Am. Assoc. Petroleum Geologists Bull., v. 60, no. 4, p. 554-565.

Mast, R. F., 1967, The development of a reservoir data system with examples of its application in Illinois: Interstate Oil Compact Comm. Committee Bulletin, v. 9, no. 1, p. 21-28; Illinois Geol. Survey Reprint Series 1967-N.

McCord, C. D., 1957, Medicine Hat gas field: Alberta Soc. Petroleum Geologists, 7th Ann. Field Conference Guidebook, p. 142-145.

McGinnis, L. D., 1968, Glaciation as a possible cause of mineral deposition: Econ. Geology, v. 63, p. 390-400.

Meents, W. F., A. H. Bell, O. W. Rees, and W. G. Tilbury, 1952, Illinois oil field brines: their geologic occurrence, and chemical deposition: Illinois Geol. Survey Illinois Petroleum, no. 66, 38 pp.

Meyboom, P., 1960, Milk River Sandstone: Alberta Research Council, Memo 2, 89 pp.

Miller, D., R. A. Bauer, and R. Johnson, 1980, Physical Properties, [in] Geologic and geochemical studies of the New Albany Shale Group (Devonian-Mississippian) in Illinois, R. E. Bergstrom, N. F. Shimp, and R. M. Cluff: Illinois Geol. Survey Final Report prepared for U.S. Dept. of Energy under contract No. DE-AC21-76ET12142, p. 77-94.

Neuman, S. P., and P. A. Witherspoon, 1969, Applicability of current theories of flow in leaky aquifers: Water Resour. Res., v. 5, no. 4, p. 817-829.

Penner, D. G., 1958, Mississippian stratigraphy of southern Alberta plains, in Goodman, A. J. (editor), Jurassic and Carboniferous of Western Canada--a symposium: Am. Assoc. Petroleum Geologists, John Andrew Allen Memorial Volume, p. 260-288.

Pettijohn, F. J., 1957, Sedimentary rocks: Harper and Brothers, New York, 718 pp.

Pratt, H. R., G. Zandt, and M. Bouchon, 1979, Earthquake related displacement fields near underground facilities: U.S. Dept. of Energy, DP-1533, 65 pp.

Rubey, W. W., 1930, Lithologic studies of fine-grained Upper Cretaceous sedimentary rocks of the Black Hills region: U.S. Geol. Survey Prof. Paper 165A, p. 1-54.

Russell, W. L., 1928, The origin of artesian pressure: Econ. Geology, v. 23, p. 132-157.

Schoon, R. A., 1971, Geology and hydrology of the Dakota Formation in South Dakota: South Dakota Geol. Survey Report of Inv. 104, 55 pp.

Schoon, R. A., and D. J. McGregor, 1974, Geothermal potentials in South Dakota: South Dakota Geol. Survey Report of Inv. 110, 76 pp.

Schultz, L. G., 1978, Mixed-layer clay in the Pierre Shale and equivalent rocks, Northern Great Plains Region: U.S. Geol. Survey Prof. Paper 1064-A, 28 pp.

Schwartz, F. W., 1975, Hydrogeologic investigation of a waste management site in southern Alberta: Can. Geotechnical Jour., v. 12, no. 3, p. 349-361.

Schwartz, F. W., and K. Muehlenbachs, 1979, Isotope and ion geochemistry of groundwaters in the Milk River Aquifer, Alberta: Water Resour. Res., v. 15, no. 2, p. 259-268.

Schwartz, F. W., and A. S. Crowe, 1980, A deterministic-probabilistic model for contaminant transport: U.S. Nuclear Regulatory Comm., NUREG/CR-1609, 158 pp.

Schwartz, F. W., and F. A. Donath, 1980, Scenario development and evaluation related to the risk assessment of high level radioactive waste repositories: U.S. Nuclear Regulatory Comm., NUREG/CR-1608, 86 pp.

Schwartz, F. W., K. Muehlenbachs, and D. W. Chorley, 1980, Flow system controls on the chemical evolution of groundwater: in press, Proc., 26th International Geological Congress.

Searight, W. V., 1937, Lithologic stratigraphy of the Pierre Formation of the Missouri Valley in South Dakota: South Dakota Geol. Survey Report of Inv. 27, 63 pp.

Shepard, J. H., 1895, The artesian waters of South Dakota: South Dakota Agr. College and Exp. Sta., Bull. 41, 76 pp.

Shurr, G. W., 1977, The Pierre Shale, northern Great Plains: a potential isolation medium for radioactive waste: U.S. Geol. Survey Open File Report 77-776, 27 pp.

Skinner, B. J., 1966, Thermal expansion, in Handbook of Physical Constants, S. P. Clark (Ed.), Geol. Soc. of America Memoir 97, p. 75-96.

Stevenson, D. L., and D. R. Dickerson, 1969, Organic geochemistry of the New Albany Shale in Illinois: Illinois Geol. Survey Illinois Petroleum 90, 11 pp.

Swanson, V. E., 1961, Geology and geochemistry of uranium in marine black shales: U.S. Geol. Survey Prof. Paper 356-C, p. 67-112.

Swenson, F. A., 1968, New theory of recharge to the artesian basin of the Dakotas: Geol. Soc. of America Bull., v. 79, p. 163-182.

Sykes, J. F., 1980, Modeling of potassium migration from the Borden landfill: EOS, v. 61, no. 17, p. 232.

Tamura, T., 1972, Sorption phenomena significant in radioactive-waste disposal: American Assoc. Petroleum Geol. Memoir 18, p. 318-330.

Thompson, R. L., and M. B. B. Crockford, 1958, The Jurassic subsurface in southern Alberta, in Goodman, A. J. (editor), Jurassic and Carboniferous of Western Canada--a symposium: Am. Assoc. Petroleum Geologists, John Andrew Allen Memorial Volume, p. 52-64.

Tóth, J., 1962, A theory of ground-water motion in small drainage basins in central Alberta, Canada: Jour. Geophys. Res., v. 67, p. 4375-4387.

Tóth, J., 1963, A theoretical analysis of ground-water flow in small drainage basins: Jour. Geophys. Res., v. 68, p. 4795-4812.

Tourtelot, H. A., 1962, Preliminary investigation of the geologic setting and chemical composition of the Pierre Shale, Great Plains region: U.S. Geol. Survey Prof. Paper 390, 74 pp.

Tourtelot, H. A., L. G. Schultz, and J. R. Gill, 1960, Stratigraphic variations in mineralogy and chemical composition of the Pierre Shale in South Dakota and adjacent parts of North Dakota, Nebraska, Wyoming, and Montana: U.S. Geol. Survey Prof. Paper 400-B, p. B447-B452.

Tovell, W. M., 1958. The development of the Sweetgrass Arch, southern Alberta: Geol. Assoc. Canada Proc., v. 10, p. 19-20.

Van Den Berg, J., 1980, Petroleum industry in Illinois, 1978: Illinois Geol. Survey, Illinois Petroleum 116, 132 pp.

Wahi, K. K. et al., 1980, Numerical simulations of earthquake effects on tunnels for generic nuclear waste repositories: U.S. Dept. of Energy, DP-1579, 130 pp.

Walton, W. C., 1960, Leaky artesian aquifer conditions in Illinois: Illinois Water Survey Report of Inv. 39, 27 pp.

Walton, W. C., and Sandor Csallany, 1962, Yields of deep sandstone wells in northern Illinois: Illinois Water Survey Report of Inv. 43, 47 pp.

Webb, J. B., 1951, Geological history of the plains of Western Canada: Am. Assoc. Petroleum Geologists Bull., v. 35, p. 2291-2315.

Weir, J. D., 1949, Marine Jurassic formations of southern Alberta plains: Am. Assoc. Petroleum Geologists Bull., v. 33, no. 4, p. 547-563.

Willman, H. B., and J. C. Frye, 1970, Pleistocene stratigraphy of Illinois: Illinois Geol. Survey Bull. 94, 204 pp.

Willman, H. B. et al., 1975, Handbook of Illinois Stratigraphy: Illinois Geol. Survey Bull. 95, 261 pp.

Workman, L. E., 1958, Glauconitic sandstone in southern Alberta: Jour. Alberta Soc. Petroleum Geologists, v. 6, no. 10, p. 237-245.

APPENDIX

DATA FOR SIMULATING GROUND-WATER FLOW AND CONTAMINANT TRANSPORT IN THE REFERENCE REPOSITORY SYSTEM IN SHALE

The data necessary to model the reference repository in shale are presented in this appendix. A detailed discussion of the geological cross section, the grid imposed over the area and the variation in hydraulic conductivity has been presented previously in Section 3. Unless otherwise stated all units are metric (m, days, gm, meq).

The following data set is used to produce one of the simulations presented in Section 4. Readers can refer to Schwartz and Crowe (1980) for a more detailed discussion of particular parameters and information concerning the format.

CROSS-SECTION SUMMARY

NUMBER OF ROWS:	27	NUMBER OF HORZ. CONDUCTIVITY UNITS:	8
NUMBER OF COLUMNS:	61	NUMBER OF VERT. CONDUCTIVITY UNITS:	8
HORZ. NODE SPACING:	2413.0	NUMBER OF LONG. DISPERSIVITY UNITS:	1
VERT. NODE SPACING:	45.7	NUMBER OF DIFFERENT POROSITY UNITS:	1
		NUMBER OF DIFFERENT C.E.C. UNITS:	1
		NUMBER OF CONSTANT HEAD NODES:	161

CONTAMINANT PARAMETERS

RADIOACTIVE HALF-LIFE:	-1.00	NUMBER OF STEPS BETWEEN LISTINGS:	5
NUMBER OF STEPS IN TIME:	20	TOTAL CONCENTRATION IN SOLUTION:	0.1000
BULK DENSITY OF MEDIUM:	1.00	SELECTIVITY COEFFICIENT FOR EXCHANGE:	0.0
SIZE OF TIME-STEP:	7300000.00	INITIAL MASS ADDED PER PART:	16540000.000

NUMBER OF PARTICLES ADDED TO THE SYSTEM PER TIME-STEP

ROW	COLUMN	PARTICLES ADDED PER STEP															
16	51	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100	100
		100	100	100	100	100											

ROW AND COLUMN NUMBERS OF THE WATER TABLE

COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW
1	21	2	21	3	21	4	21	5	22	6	22	7	22	8	22	9	22	10	22
11	22	12	22	13	22	14	22	15	22	16	22	17	22	18	22	19	22	20	22
21	22	22	23	23	23	24	23	25	23	26	23	27	23	28	23	29	23	30	23
31	24	32	24	33	24	34	24	35	24	36	24	37	24	38	24	39	24	40	24
41	24	42	24	43	24	44	25	45	25	46	25	47	25	48	25	49	25	50	25
51	25	52	26	53	26	54	26	55	26	56	26	57	26	58	27	59	27	60	27
61	27																		

ROW AND COLUMN NUMBERS OF THE BOTTOM BOUNDARY

COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW	COL	ROW
1	1	2	1	3	1	4	1	5	1	6	1	7	1	8	1	9	1	10	1
11	1	12	2	13	2	14	2	15	2	16	2	17	2	18	2	19	2	20	2
21	2	22	2	23	3	24	3	25	3	26	3	27	3	28	3	29	3	30	3
31	3	32	3	33	3	34	3	35	3	36	3	37	3	38	3	39	3	40	3
41	3	42	3	43	3	44	3	45	3	46	4	47	4	48	4	49	4	50	4
51	5	52	5	53	5	54	5	55	5	56	5	57	6	58	6	59	6	60	6
61	6																		

NOTE: The numbering convention used here places Row 1 and Column 1 in the lower left hand corner of the grid.

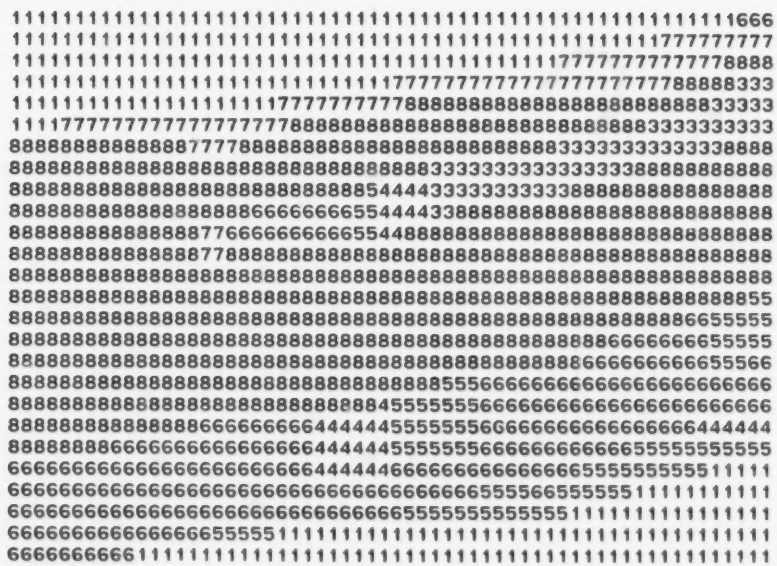
CONSTANT HEAD VALUES (HEAD VALUES IN METERS A.M.S.L.)

COL	ROW	HEAD	COL	ROW	HEAD	COL	ROW	HEAD	COL	ROW	HEAD	COL	ROW	HEAD	COL	ROW	HEAD
1	1	884.	1	2	884.	1	3	884.	1	4	884.	1	5	884.	1	6	884.
1	7	874.	1	8	864.	1	9	854.	1	10	844.	1	11	834.	1	12	824.
1	13	815.	1	14	806.	1	15	798.	1	16	792.	1	17	784.	1	18	776.
1	19	766.	1	20	758.	1	21	750.	2	21	755.	3	21	763.	4	21	771.
5	22	780.	6	22	777.	7	22	774.	8	22	772.	9	22	770.	10	22	769.
11	22	768.	12	22	767.	13	22	766.	14	22	758.	15	22	750.	16	22	740.
17	22	730.	18	22	750.	19	22	770.	20	22	790.	21	22	810.	22	23	820.
23	23	830.	24	23	835.	25	23	840.	26	23	844.	27	23	848.	28	23	852.
29	23	885.	30	23	860.	31	24	864.	32	24	864.	33	24	868.	34	24	870.
35	24	872.	36	24	874.	37	24	875.	38	24	877.	39	24	880.	40	24	883.
41	24	886.	42	24	895.	43	24	905.	44	25	915.	45	25	925.	46	25	930.
47	25	934.	48	25	937.	49	25	940.	50	25	944.	51	25	948.	52	26	952.
53	26	955.	54	26	957.	55	26	958.	56	26	959.	57	26	960.	58	27	972.
59	27	984.	60	27	995.	61	27	1000.	61	26	999.5	61	25	999.	61	24	998.
61	23	997.	61	22	996.8	61	21	996.6	61	20	996.4	61	19	996.	61	18	995.
61	17	994.	61	16	993.	61	15	992.	61	14	991.	61	13	990.7	61	12	990.6
61	11	990.5	61	10	990.4	61	9	990.3	61	8	990.2	61	7	990.1	61	6	990.
60	6	990.	59	6	988.	58	6	986.	57	6	984.	56	5	982.	55	5	981.
54	5	980.	53	5	979.	52	5	976.	51	5	973.	50	4	970.	49	4	967.
48	4	964.	47	4	961.	46	4	958.	45	3	955.	44	3	952.	43	3	950.
42	3	948.	41	3	946.	40	3	944.	39	3	942.	38	3	940.	37	3	938.
36	3	936.	35	3	934.	34	3	932.	33	3	930.	32	3	928.	31	3	926.
30	3	924.	29	3	922.	28	3	920.	27	3	918.	26	3	917.	25	3	916.
24	3	915.	23	3	914.	22	2	913.	21	2	912.	20	2	911.	19	2	910.
18	2	909.	17	2	908.	16	2	907.	15	2	906.	14	2	905.	13	2	904.
12	2	903.	11	1	902.	10	1	901.	9	1	900.	8	1	898.	7	1	896.
6	1	894.	5	1	892.	4	1	890.	3	1	898.	2	1	896.			

HORIZONTAL CONDUCTIVITY LEGEND (M/DAY)

1	0.0
2	0.4320E+02
3	0.4320E+01
4	0.4320E+00
5	0.4320E-01
6	0.4320E-02
7	0.4320E-03
8	0.4320E-04

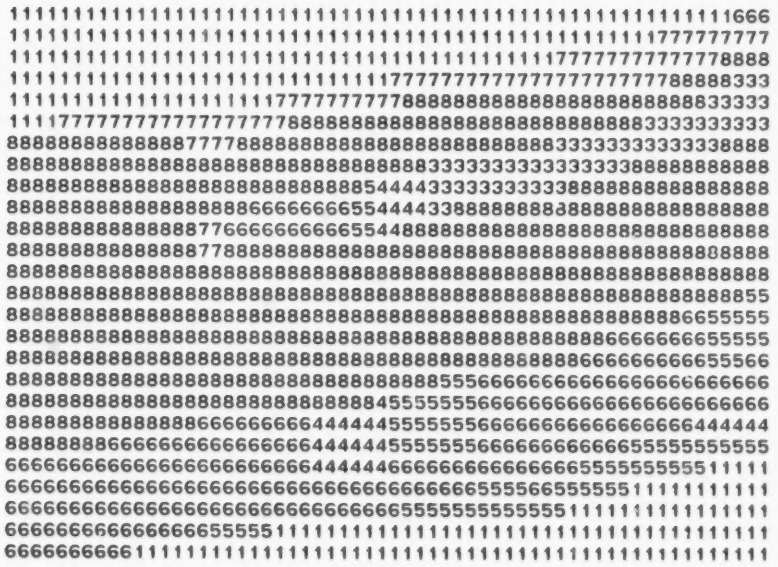
HORIZONTAL CONDUCTIVITY CODE



VERTICAL CONDUCTIVITY LEGEND (M/DAY)

1	0.0
2	0.8640E+01
3	0.8640E+00
4	0.8640E-01
5	0.8640E-02
6	0.8640E-03
7	0.8640E-04
8	0.8640E-05

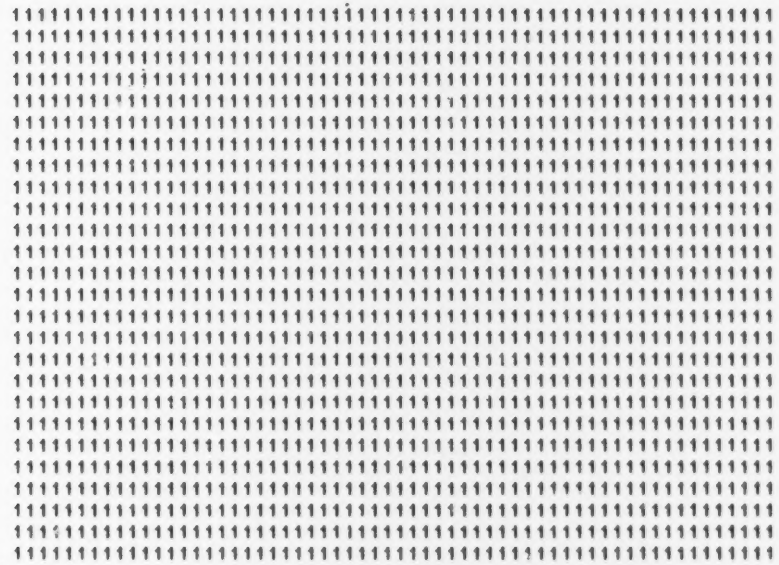
VERTICAL CONDUCTIVITY CODE



LONGITUDINAL DISPERSIVITY LEGEND (M)

0.3000E+01

LONGITUDINAL DISPERSIVITY CODE

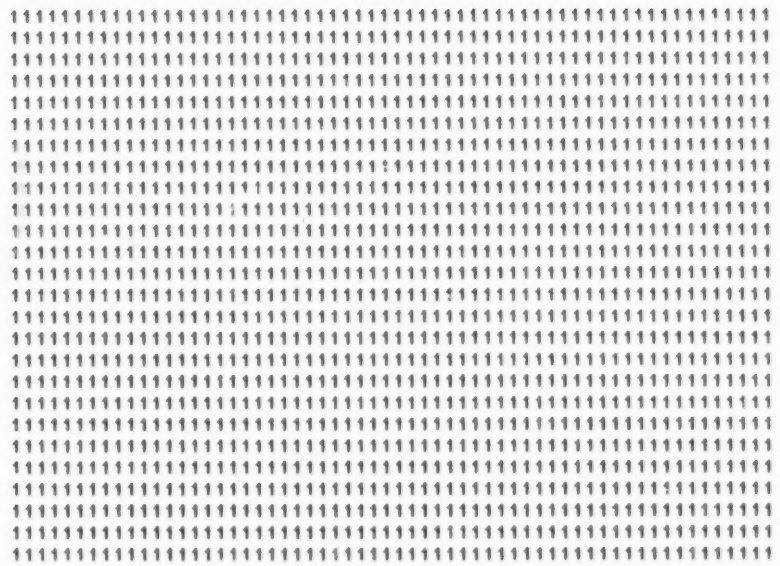


NOTE: Inasmuch as the contaminants were not tracked out of the host unit, dispersivity in the other units is not of concern for the transport simulations presented.

POROSITY LEGEND

1 0.1500E+00

POROSITY CODE

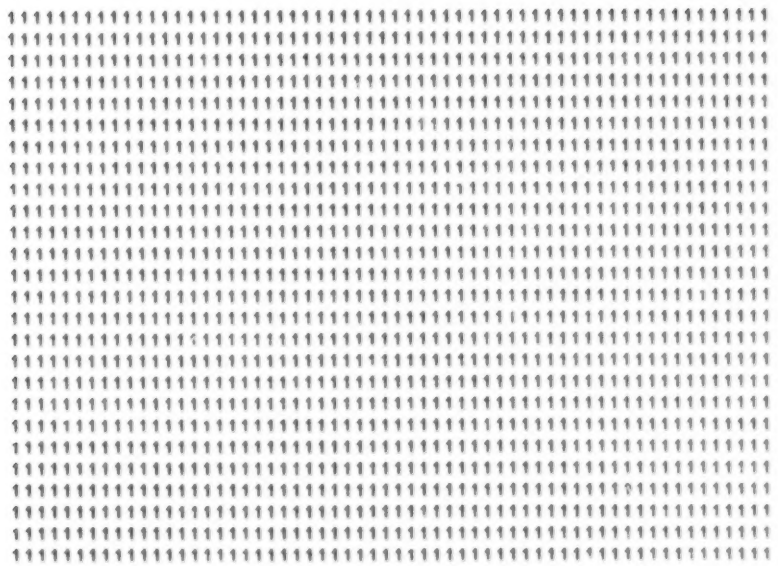


NOTE: Inasmuch as the contaminants were not tracked out of the host unit, porosity in the other units is not of concern for the transport simulations presented.

CATION EXCHANGE CAPACITY LEGEND (MEQ/GM)

1 0.1000E+00

CATION EXCHANGE CAPACITY CODE



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